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

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*EPFL +INRIA and ENS Paris

Supervised learning with neural networks

Prediction/classification task

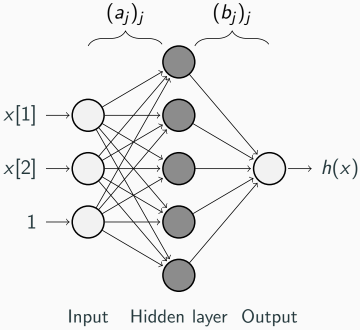
- Couple of random variables (X, Y) on $\mathbb{R}^d \times \mathbb{R}$
- Given n i.i.d. samples $(x_i, y_i)_{i=1}^n$, build h s.t. $h(X) \approx Y$

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



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

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

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

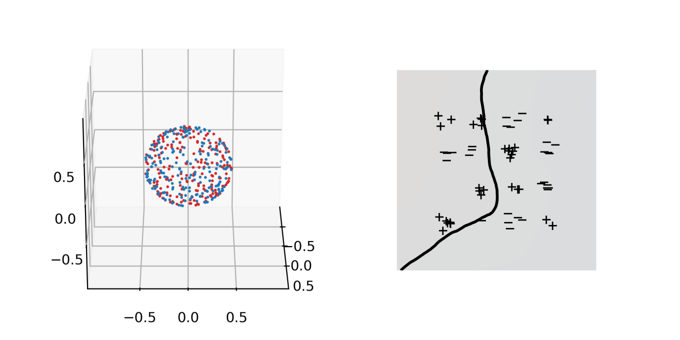
Gradient flow

- 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 : logistic loss, unregularized ($\lambda = 0$)



Space of parameters

- plot $|b_j| \cdot a_j$
- color depends on sign of b_j
- 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 $h((w_j(\infty))_j, \cdot)$?

Outline

Infinite width limit: global convergence

Regularized case: function spaces

Unregularized case: implicit regularization

Infinite width limit: global convergence

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[1]

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

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 a.s. in $\mathcal{P}_2(\mathbb{R}^{d+2})$ to μ_t, the unique Wasserstein gradient flow of F starting from μ_0.

1. For ReLU, take expectations over small perturbations of the x_i.

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* μ_t *converges weakly to* μ_∞*, then* μ_∞ *is a global minimizer of* F*.*

- Initialization matters: the key assumption on μ_0 is *diversity*
- Corollary: $\lim_{m,t\to\infty} F(\mu_{m,t}) = \min F$
- Open question: convergence of μ_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: teacher student

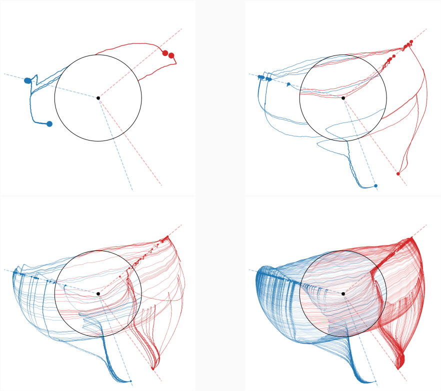


Figure 1: SGD on expected square loss, $X \sim \mathcal{U}_{\mathbb{S}^d}$ and $Y = h((w_i^*)_{i=1}^{m^*}, X)$

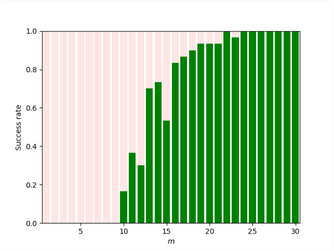


Figure 2: Success rate when $d = 100$, $m^* = 10$

[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.*

Regularized case: function spaces

Variation norm

Definition (Variation norm)

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

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

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.*

Fixing the 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

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

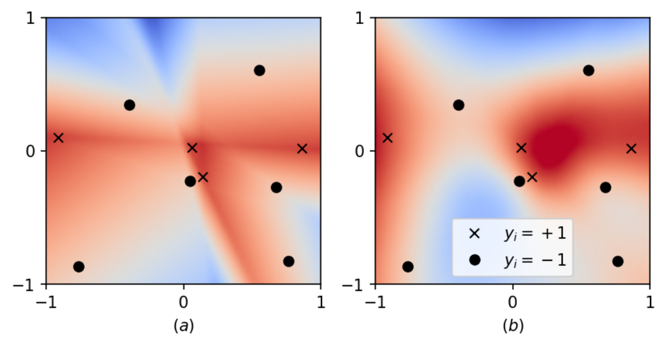
Proposition (Kernel ridge regression)

All else unchanged, fixing the hidden layer leads to minimizing

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

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)

	$\mathcal{F}_1$	$\mathcal{F}_2$
Stat. prior	**Adaptivity** to anisotropy	Isotropic smoothness
Optim.	No guarantee	**Guaranteed** efficiency

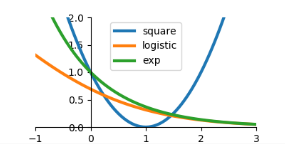
Bach (2014). *Breaking the curse of dimensionality with convex neural networks.*

Unregularized case: implicit regularization

Preliminary: linear classification with exponential loss

Classification task

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



Loss for $y = 1$

Theorem (SHNGS 2018, reformulated)

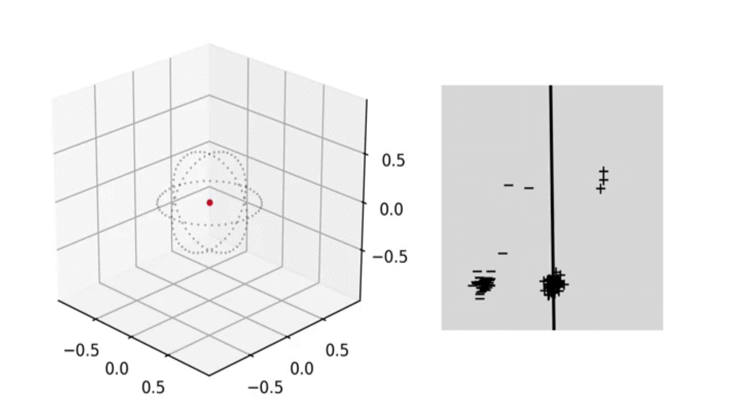
Consider $h(w, x) = w^\top x$ and a linearly separable training set. For any $w(0)$, the normalized gradient flow $\bar{w}(t) = w(t)/\|w(t)\|_2$ converges to a $\|\cdot\|_2$-max-margin classifier, i.e. a solution to

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

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

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

Implicit regularization for linear classification: illustration



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

Implicit regularizations for 2-layer neural networks

Back to wide 2-layer ReLU neural networks.

Theorem (C. & Bach, 2020)

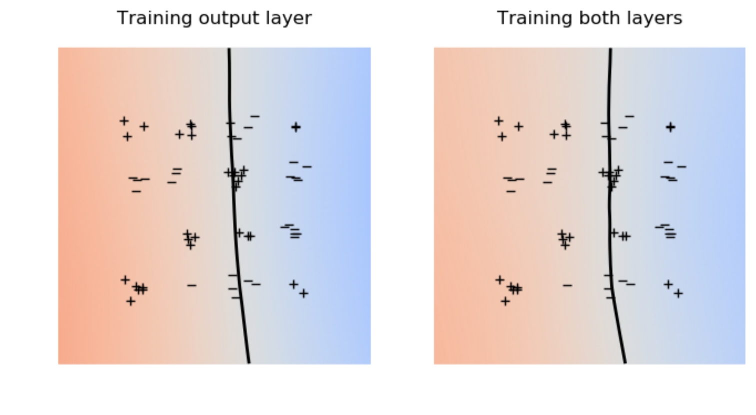
Assume that $\mu_0 = \mathcal{U}_{\mathbb{S}^d} \otimes \mathcal{U}_{\{-1,1\}}$, *that the training set is consistant* ($[x_i = x_j] \Rightarrow [y_i = y_j]$) *and technical conditions (in particular, of convergence). Then* $h(\mu_t, \cdot)/\|h(\mu_t, \cdot)\|_{\mathcal{F}_1}$ *converges to the* $\mathcal{F}_1$*-max-margin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

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

- fixing the hidden layer leads to the $\mathcal{F}_2$-max-margin classifier
- we also prove convergence speed bounds in simpler settings

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

Illustration



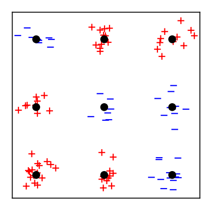
$h(\mu_t, \cdot)$ for the exponential loss, $\lambda = 0$ ($d = 2$)

Numerical experiments

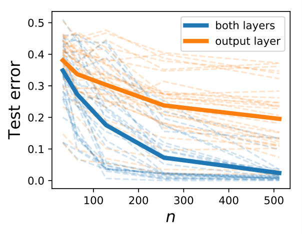
Setting

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

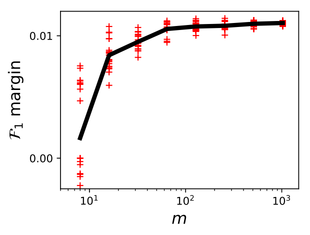
- two first coordinates as shown on the right
- all other coordinates uniformly at random



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 regularizations in one dynamics (I)

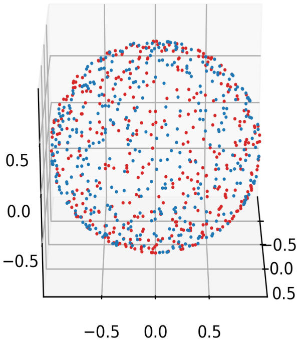
Lazy training (informal)

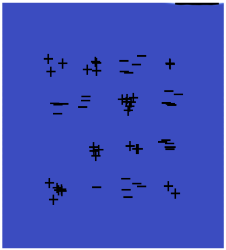
All other things equal, if the variance at initialization is large and the step-size is small then the model behaves like its first order expansion over a significant time.

- Neurons hardly move but significant total change in $h(\mu_t, \cdot)$
- 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 regularizations 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

- Open question: make statements of this talk quantitative
  - $\rightsquigarrow$ how fast is the convergence ? how many neurons are needed?
- Mathematical models for deeper networks
  - $\rightsquigarrow$ goal: formalize training dynamics & study generalization

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[Talk based on the following papers:]

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

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 π_r?

Theorem (Bach '14, reformulated)

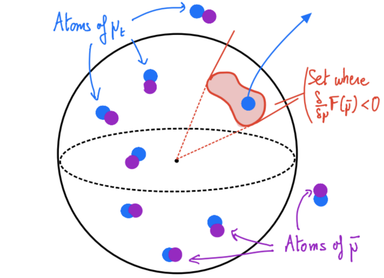
For a suitable choice of regularization $\lambda(n) > 0$, the minimizer of F with square loss enjoys an error bound in $\tilde{O}(n^{-1/(r+3)})$.

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

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

Proof Intuition (Global Convergence Thm.)

- Using homogeneity & convexity, μ^* minimizes F iff
  (i) $\frac{\delta}{\delta\mu}F(\mu^*)[w] = 0$, for μ^*-a.e w ($\Leftarrow$ stationary point of PDE)
  (ii) $\frac{\delta}{\delta\mu}F(\mu^*)[w] \geq 0$
- If μ_0 has mass in all directions, so does μ_t for any $t \geq 0$
- If $\bar{\mu}$ does not satisfy (ii), then μ_t cannot be trapped near $\bar{\mu}$



- Thus if μ_t converges, its limit is a minimizer of F by (i) & (ii)