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

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Supervised learning with neural networks

Supervised machine learning

- Consider a 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 such that $h(X) \approx Y$

Wide 2-layer ReLU neural networks

Class of predictors h of the form, for some large *width* $m \in \mathbb{N}$,

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

where $\phi(w, x) := c \max\{a^\top x + b, 0\}$ and $w := (a, b, c) \in \mathbb{R}^{d+2}$.

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

Learning algorithm: selects $(w_j)_j$ using the training data

Gradient flow of the empirical risk

Empirical risk minimization

- Choose a loss $\ell : \mathbb{R}^2 \to \mathbb{R}$ convex & smooth in its 1st variable
- "Minimize" the empirical risk with a regularization $\lambda \geq 0$

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

Gradient-based learning

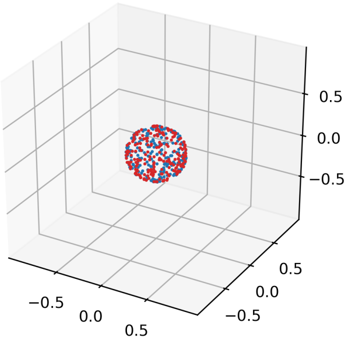
- Initialize $w_1(0), \ldots, w_m(0) \overset{\text{i.i.d}}{\sim} \mu_0 \in \mathcal{P}_2(\mathbb{R}^{d+2})$
- Decrease the non-convex objective via gradient flow, for $t \geq 0$,

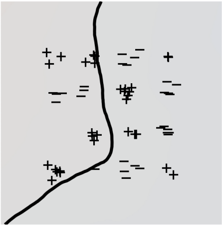
$$\frac{\mathrm{d}}{\mathrm{d}t}(w_j(t))_j = -m\nabla F_m((w_j(t))_j)$$

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

Illustration

Dynamics for a classification task: unregularized logistic loss, $d = 2$





Space of parameters

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

Space of predictors

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

Motivations

Main question

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

- Understanding 2-layer networks: when are they powerful?
  - $\rightsquigarrow$ role of initialization μ_0, loss, regularization, data structure, etc.
- Understanding representation learning via back-propagation
  - $\rightsquigarrow$ not captured by current theories for deeper models who study perturbative regimes around the initialization
- Natural next theoretical step after linear models
  - $\rightsquigarrow$ we can't understand the deep if we don't understand the shallow
- Beautiful connections with rich mathematical theories
  - $\rightsquigarrow$ variation norm spaces, Wasserstein gradient flows

Outline

Global convergence in the infinite width limit

Generalization with regularization

Implicit bias in the unregularized case

Global convergence in the infinite width limit

Wasserstein gradient flow formulation

- 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

$$\mathrm{spt}(\mu_0) \subset \{|c|^2 = \|a\|_2^2 + |b|^2\}.$$

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 μ_t, the unique Wasserstein gradient flow of F starting from μ_0.

[Refs]:
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 $\mu_0 = \mathcal{U}_{\mathbb{S}^d} \otimes \mathcal{U}_{\{-1,1\}}$. If μ_t converges to μ_∞ in $\mathcal{P}_2(\mathbb{R}^{d+2})$, then μ_∞ is a global minimizer of F.

- Initialization matters: the key assumption on μ_0 is *diversity*
- Corollary: $\lim_{m,t\to\infty} F(\mu_{m,t}) = \min F$
- Convergence of μ_t: open question (even with compactness)

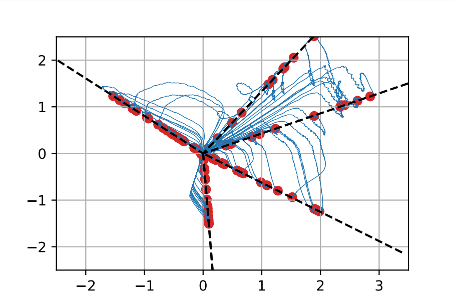
Generalization bounds?

They depend 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)

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

Illustration: population risk



Stochastic gradient descent on population risk ($m = 100$, $d = 1$)

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)

Square loss $\ell(y, y') = (y - y')^2$.

[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.*

Generalization with regularization

Variation norm

Definition (Variation norm)

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

$$\begin{aligned}\|h\|_{\mathcal{F}_1} &:= \min_{\mu \in \mathcal{P}_2(\mathbb{R}^{d+2})} \left\{ \frac{1}{2} \int \|w\|_2^2 \, \mathrm{d}\mu(w) \; ; \; h(x) = \int \phi(w,x) \, \mathrm{d}\mu(w) \right\} \\ &= \min_{\nu \in \mathcal{M}(\mathbb{S}^d)} \left\{ \|\nu\|_{TV} \; ; \; h(x) = \int \max\{a^\top x + b, 0\} \, \mathrm{d}\nu(a,b) \right\}\end{aligned}$$

Proposition

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

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

[Refs]:

Neyshabur, Tomioka, Srebro (2015). *Norm-Based Capacity Control in Neural Networks.*

Kurkova, Sanguineti (2001). *Bounds on rates of variable-basis and neural-network approximation.*

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 $\ell(y, y') = (y - y')^2$ 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

[Refs]:
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 $(a, b)\}$

Definition (Conjugate RKHS)

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

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

Proposition (Kernel ridge regression)

All else unchanged, fixing the hidden layer leads to minimizing

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

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

Implicit bias in the unregularized case

Preliminary: linear classification and exponential loss

Classification task

- $Y \in \{-1, 1\}$ and the prediction is $\text{sign}(h(X))$
- $\ell(y, y') = \exp(-y'y)$ or logistic $\ell(y, y') = \log(1 + \exp(-y'y))$
- 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

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

[Refs]:
Soudry, Hoffer, Nacson, Gunasekar, Srebro (2018). *The Implicit Bias of Gradient Descent on Separable Data*.
Telgarsky (2013). *Margins, shrinkage, and boosting*.

Interpretation as online optimization

- look at $w'(t) = \nabla F_1(w(t))$, where F_β is the *smooth-margin*:

$$F_\beta(w) = -\frac{1}{\beta}\log\left(\frac{1}{n}\sum_{i=1}^{n}\exp(-\beta y_i \cdot w^\intercal x_i)\right) \xrightarrow[\beta\to\infty]{} \min_i y_i \cdot w^\intercal x_i$$

- prove that $\|w(t)\| \to \infty$ if the training set is linearly separable
- denoting $\bar{w}(t) = w(t)/\|w(t)\|_2$, it holds

$$\frac{d}{dt}\bar{w}(t) = \frac{1}{\|w(t)\|}\nabla F_{\|w(t)\|}(\bar{w}(t)) - \alpha_t \bar{w}(t)$$

  for some $\alpha_t > 0$ that constraints $\bar{w}(t)$ to the sphere
- "thus" $\bar{w}(t)$ performs online projected gradient ascent on the sequence of objectives $F_{\|w(t)\|}$ which converge to the margin.

Implicit bias of two-layer neural networks

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

Theorem (C. & Bach, 2020)

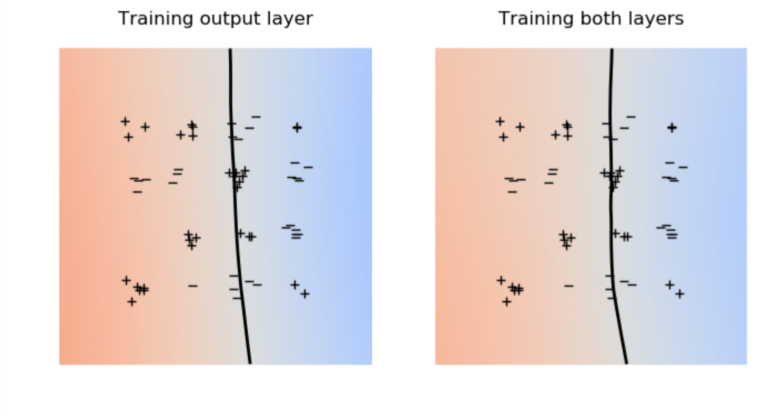
Assume that $\mu_0 = \mathcal{U}_{\mathbb{S}^d} \otimes \mathcal{U}_{\{-1,1\}}$, *that the training set is consistant* ($[x_i = x_j] \Rightarrow [y_i = y_j]$) *and that* μ_t *and* $\nabla F(\mu_t)$ *converge in direction (i.e. after normalization). Then* $h(\mu_t, \cdot)/\|h(\mu_t, \cdot)\|_{\mathcal{F}_1}$ *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

[Refs]:
Chizat, Bach. *Implicit Bias of Gradient Descent for Wide Two-layer Neural Networks [...].*

Illustration



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

Statistical efficiency

Assume that $\|X\|_2 \leq R$ 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),

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

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

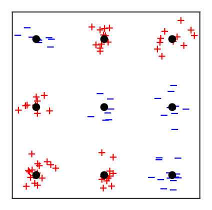
[Refs]:
Chizat, Bach. *Implicit Bias of Gradient Descent for Wide Two-layer Neural Networks [...].*

Numerical experiments

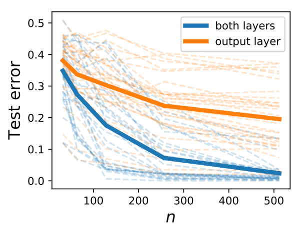
Setting

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

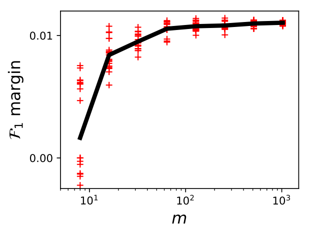
- two first coordinates as shown on the right
- all other coordinates uniformly at random



Coordinates 1 & 2



(a) Test error vs. n



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

Two implicit biases in one dynamics (I)

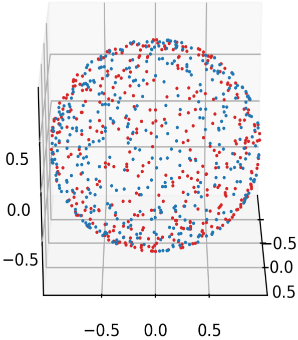
Lazy training (informal)

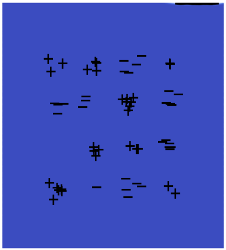
All other things equal, if the variance at initialization is large and the step-size is small then the model behaves like its first order expansion over a significant time.

- 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

[Refs]:
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**

Conclusion

- **Generalization guarantees for gradient methods on neural nets**
- **Analysis via Wasserstein gradient flow with homogeneity**

Perspectives

- **Proof of convergence, quantitative results**
- **More complex architectures**

[Papers :]

- Chizat and Bach (2018). On the Global Convergence of Over-parameterized Models using Optimal Transport
- 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/