GOING BEYOND THE LINEAR REGIME

- 1) Trackelitity via overparemetrizato
- 2) Double descent 3) Benign overfitting as NNs (self-induced - A Separation between linearized NNs regularzation)
- B) Essed features us feature learning:
 breaking the curre of dimensionally using feature barning
- -> © An example : learning parities
- ___ D Moth approaches beyond linear regime

1 Separation between linearized NNs is NNs

LINEAR REGIME: training regime where network can be approximated by a linear model during the whole training dynamics

$$\Rightarrow \beta(\alpha, \Theta) \longleftrightarrow \beta^{lin}(\alpha, \Theta) = \beta(\alpha, \Theta_0) + \langle \Theta - \Theta_0, \frac{\nabla \beta(\alpha, \Theta_0)}{\Theta} \rangle$$

$$\Theta^{\circ} = \overline{\Theta}^{\circ} = \Theta_{\circ}$$

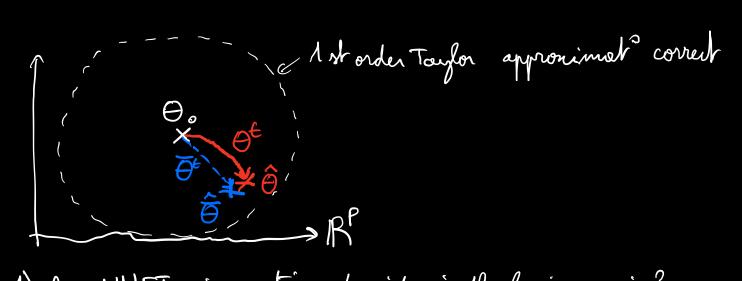
$$\mathbf{O} \dot{\mathbf{O}}^{\epsilon} = -\nabla \hat{R}_{m} (f(\mathbf{x}, \mathbf{O}^{\epsilon}))$$

$$\hat{\Theta}^{t} = - \nabla \hat{R}_{n}(\hat{\beta}^{lin}(x, \bar{\Theta}^{t}))$$

$$\| \Theta^{t} - \overline{\Theta}^{t} \|_{2} << 1$$

$$\Rightarrow$$
 $\beta(\alpha, \Theta^{t}) \approx \beta^{lin}(\alpha, \overline{\Theta}^{t})$

=> in this regime: NNETs can effectively be replaced by linear models



- 1) Are NNETs in practice kramed in the linear regime?

 -> Sometimes, mostly not.
- 2) Does linear theory capture what can be achieved by NNETs?

 No.
- 3) Do we have a better theory? -> understand both optimisation -> Not yet. and generalization.

Linear regime: -> explains why GD/SGD con find a globel optima of a highly non-cowen problem

Successfully illustrated: TRACTABILITY VIA OVERPARAMETRIZATION

-> problem becomes more tractable as # of parameters 7

=> since When: lots of work to show the limitation of linear regime theory to explain good generalization of NNETS

Most of the (theoretical) work: show in specific examples that NNETs outperform linearized NNETs.

This results are colled "seperation results!"

"Obrious" seperetion en approximation power:

2-layer NNET: $f(\alpha, \alpha, W) = \sum_{i=1}^{N} a_i f(\alpha_i, \alpha_i)$

a; ER, w; ER

2-layer lineained NNET: fin W° = (w, , ..., w, °)

also opply (RF) $\int_{RF} (\alpha, \alpha) = \sum_{i=1}^{N} \alpha_i \, 6(\langle \omega_i^{\circ}, \alpha_i \rangle) \int_{\text{linearizat}}^{\text{full}}$

* $F_{NN}(B) = \{ G_{NN}(a, W) : \|a\|_{2}, \|W\|_{F} \in \mathbb{B} \}$

* FRF (W°) = { GRF(a,a): a e IR N}

Approximation error: RAM (b., F) = inf || f. - b||_2 feF

Les best you can hope for ong number of samples
Take: ox a Unif (Sd-1) wio ~ Unif (Sd-1) fined best degree-l polition.
In: [Mixiahienrix et al., 2019] For any $f \in l^2(S^d)$. If $d^2 \ll N \ll d^{2+1}$, When $R_{app}(f_*, F_{RF}(W^\circ)) = P_{>l}f_* _{l^2}^2 + o_{l}(1).$
d' d' d' long (d)
Simple example: one neuron $f_*(x) = 6(\langle \omega_*, \alpha_* \rangle)$ App. with RF: $R_{App}(f_*, F_{RF}) \approx \ F_{l} G\ _{L^2}^2$ if $N \times d^2$
App- with NNETs: Rapp (be, FNN) = 0 for N21. Ls singly take $a_1 = 1$, $\omega_1 = \omega_*$ + rest set to 0
=> FNN much richer class of fets

Intuition: in high	-dim, sup ielN)) using «(Ew;	$(<\omega_i^{\circ},\omega_{\star})$	>) 2 1	
- no good feeti	re 6 (< wi, c	x) to appro	ximate $6(<\omega,$	(مر >)
- when 1st laye		can select c	good features	
		(ie. car)	high correlativith	(U.,)

Kind of obvious and not interesting: the fact that you can exproximate does not mean that you can efficiently find these good networks.

Went a reportion between linearized ANETS and NNETS. What can be "constructed in practice, e.g., using GD.

Separation between linearized NNETs and gradient brained NNETs:

Inner-Prod kernel: "infinite -width" linearized NNET $\frac{1}{N} \stackrel{N}{\underset{i=1}{\sum}} 6(\alpha, \omega;) 6(\alpha, \omega;) = \frac{1}{N} \left[\frac{1}{N} \left(\frac{1}{N}$

Test error of KRR (more details later about Kamel)

Take:
$$n \sim Unif (S^{d,n})$$
 | $e \in L^2(S^{d,n})$

Take: $n \sim Unif (S^{d,n})$ | $e \in L^2(S^{d,n})$

The dec $n \ll d^{l+1}$ (now # training somples)

Then [Minohiewicz et al., 2019]

Robber, G_{a}) = $IP_{>0}$ | $f \approx I_{12}^{2} + o_{d}(I)$

Skrainese descent

Lagain: G_{s} (α) = G (C_{s} , α)

Hen G_{s} (G_{s}) G_{s} | G

- = In general, Mudying NNETs trained by GD is currently out of reach except in the linear regime.
- => Con we understand the benefit of training more abstractly?

- Kemel
$$\frac{1}{N} \stackrel{N}{\underset{i=1}{\stackrel{\sim}{=}}} 6(\langle \omega_i^{\circ}, \alpha_i \rangle) 6(\langle \omega_i^{\circ}, \gamma_i \rangle) = \underbrace{H_0(\alpha_i \gamma_i)}_{N}$$

$$\beta_{NN}(\alpha, \Theta^t) = \sum_{i=1}^{N} \alpha_i^{\epsilon} \delta(\langle \omega_i^{\epsilon}, \alpha \rangle)$$

$$\longrightarrow \text{"Kenel": } \frac{1}{N} \underset{i=1}{\overset{N}{\geq}} 6(\langle \omega_i^{\epsilon}, \alpha_i \rangle) 6(\langle \omega_i^{\epsilon}, \alpha_i \rangle) = \underbrace{H_{\epsilon}(\alpha_i, \alpha_i)}_{\epsilon = 1}$$

Je, learning "good" features adapted to the data

$$e \cdot q : \beta_{\ast} = 6 (\langle \omega_{\bullet}, \cdot \rangle) \longrightarrow \mathcal{H}_{\ast}(\alpha, \gamma) = 6 (\langle \omega_{\bullet}, \alpha \rangle) d\alpha_{\bullet}, \gamma)$$

- · Linear regime: "kernel regime", "lazy regime"
- outside linear regime: "feature learning regime"
 rich regimes

Vortly different behavior bekween fined feature (fined kernel) and methods that allow feature learning

=> they are "adaptive" and can workly outperform fined feature models.

"Breaking the curse of dimensionality using conven NVets" - Francis BACH (2017)

Background on KRR/RKMS:

 $\xi(y_i, n_i)$ $\beta_{i \leq n}$ $y_i \in \mathbb{R}$, $\alpha_i \in \mathbb{R}^d = X$

(X, P): probe space of the data covariates ε (Λ, μ): probe space of the features weights ε weights

Easturination map: 6: X × 1 -> R $(\alpha, \omega) \mapsto 6(\alpha, \omega)$ $(6eL^2(\chi \times \Pi))$

Model: $\int_{\Gamma} (x, a) = \int_{\Gamma} a(\omega) \delta(\langle \alpha, \omega \rangle) \mu(d\omega)$ - infinitely - wide 2 layers NNet with $a: \Gamma \to \mathbb{R}$ e.g. $a(\omega) = \sum_{i=1}^{N} a_i \delta_{\omega=\omega_i}$ (direc) e Hen $\beta(x, a) = \sum_{i=1}^{n} \alpha_i \delta(\alpha_i, \omega_i)$ Define norm: $\| \beta(\cdot, \alpha) \|_{\mathcal{F}_{2}} = \left(\int_{\mathcal{F}_{2}} |\alpha(\omega)|^{2} \mu(d\omega) \right)^{\frac{1}{2}}$ $= \|\alpha\|_{L^{2}} \qquad \boxed{\mathcal{F}_{2} - norm}$ $f_{2} = \{ \{(\cdot, a) \text{ such What } \| \{(\cdot, a) \|_{F_{2}} < \infty \} \}$ - Reproducing Kernel Hilbert Space (RKHS) with kernel: $K(\alpha, \beta) = \int_{\mathcal{S}} 6(\alpha, \omega) 6(\alpha, \omega) \rho(d\omega)$ Ridge Regression: $\hat{a} = \underset{a: \mathcal{R} \to \mathcal{R}}{\operatorname{argmin}} \quad \begin{cases} \sum_{i=1}^{m} (y_i - f(x_i, a))^2 + \lambda \|a\|_{L^2}^2 \end{cases}$ $(a \in L^2(\mathcal{I}))$ Kemel Ridge Regression: > comes problem in $a \in L^2(\Omega) \Rightarrow lub on <math>\infty$ le dimensional not krackable -> Trackable: celebrated representes theorem

⇒ the solution $\hat{a} \in Span \{ \varepsilon(\alpha_i, \cdot) : i \in m \}$ proof: $a \in L^2(\Lambda)$, consider subsere $V = \text{span} \{ 6(\langle \alpha_i, \rangle) : i \leq m \}$ let $a = a_V + a_L$ $\in V^{\perp}$ space orthogonal to VWe have $f(\alpha; \alpha) = \int G(\alpha; \omega) \alpha(\omega) \mu(d\omega)$ $= \langle 6(\alpha_i), \cdot \rangle, \alpha \rangle_{L^2(\mu)} = \langle 6(\alpha_i), \alpha_i \rangle_{L^2}$ and || all2 = || av ||2 + || ax ||2 $\hat{a} = \underset{i=1}{\text{argmin}} \left\{ \sum_{j=1}^{m} (y_j - \langle 6(\alpha_{i,j}), a_{i,j} \rangle)^2 + \lambda \|a_j\|_2^2 + \lambda \|a_j\|_2^2 \right\}$ $=) \hat{a}_{\perp} = 0 \quad \text{hence} \quad \hat{a} \in \text{Spen } \{ 6(\langle \alpha_i, \cdot \rangle) : i \leq m \} \square$ Closed form solution: (â = 5 c; 6(ea;) $f(n, \hat{\alpha}) = \sum_{i=1}^{m} c_i K(\alpha, \alpha_i)$ $(K(n, n_i) = \int 6(c_n, \omega) f(\alpha_i, \omega) \mu(d\omega)$ Denote $K_m = (K(x_i, x_j))_{ij \leq m} \in \mathbb{R}^m \times \mathbb{R}^m$ $\forall z (y_1, ..., y_m) \in \mathbb{R}^m$ ce IRM & ||y-Kac||2+1cTKc3 $\hat{c} = (K_m + \lambda Id)^{-1} y$

What is the performance of KRR?
-> consider G = E b. L-lipschiky?
$\operatorname{sup}_{\theta \in \mathcal{G}} R_{\text{kert}}(\theta_*, \theta_3) \simeq m^{\frac{1}{d}}$
I for the 'work case', to get error $\leq \varepsilon$ we need $m \geq \left(\frac{1}{\varepsilon}\right)^d$
CURSE OF DIMENSIONALITY
KRR is adaptive to smoothness of the function Ly smoother fets will be easier to fit
e.a.: 1) prevois theorem: No fit degree - l polynomial [
2) Gs = E & with S first derivatives bounded }
od karnel 3 sup Rhest (f=1 f3) = m = s+d & Holder proc
=) still need smoothness S to grow with d (curse of dim.)

Sad

Con we hope to do better?

- No: there clares of fets are too lig ('plague ly the curse of dim') Need to restrict to a smaller class of fet

Interesting class of fets: = a (Un)

U e Raxd

-> fets that only depend on a on a low-dimensional projection

Why?

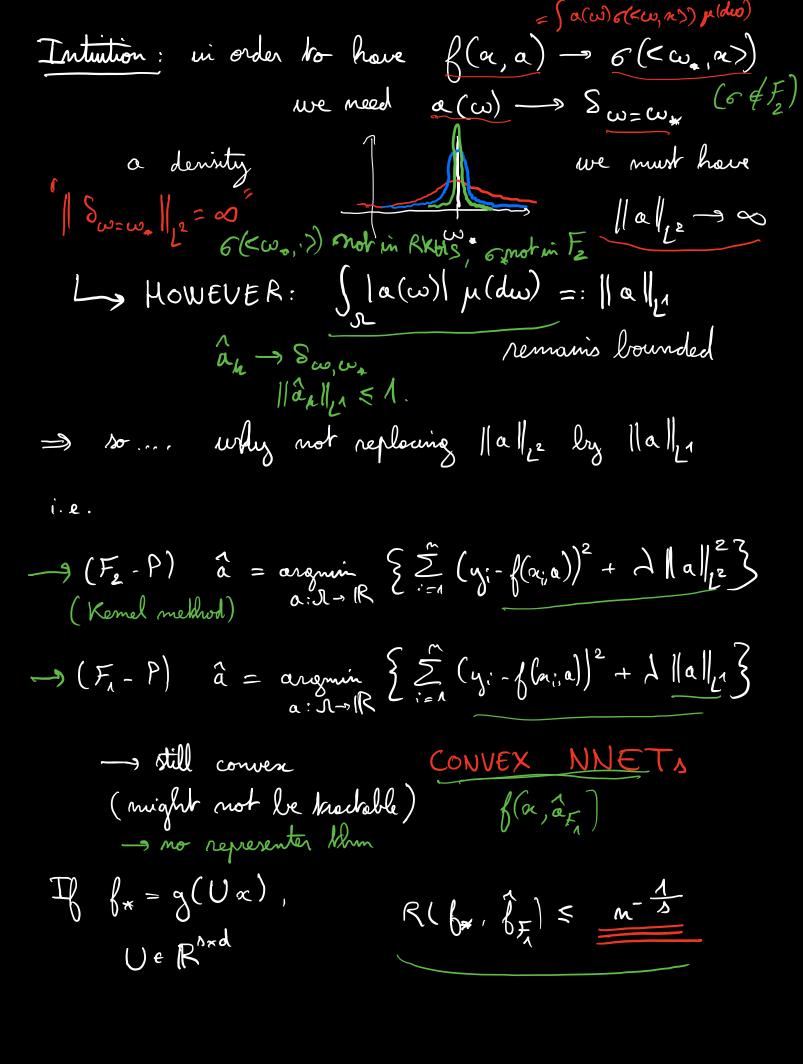
 $f(\alpha, \alpha) = \int 6(\alpha, \omega) \alpha(\omega) \mu(d\omega)$ -> put all the weights a (w) on w & In(U')

-s problem effectively s-dimensional d-s.

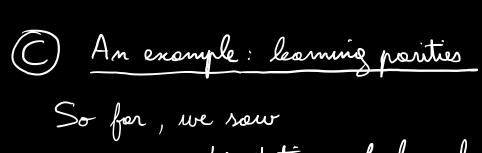
Les hope to get $O(n^{\frac{1}{5}})$ rate.

However: Kernel methods are not adaptive to fets that depend only on a low-dimensional projection of data

Recoll: Let $m \times d^2$, $R_{\text{test}}(f_0, f_0) = \|P_0 f_0\|_{L^2}^2 + o_{d}(1)$ $L_0 \quad mo \quad matter \quad \text{the structure on } f_{\text{test}}(e, g) = 6(<\omega_{\text{a}}, a)$



Conver NNets break the curse of dimensionality on fets that only depend on a low-duin projection of the date
=> adaptive to batent linear structure (U is unknown)
However Fi is not trackable (hard problem)
_s can think about GD as approximately solving F,
=) ni general do not expect GD to solve F ₁ - problems (not the right implicit bras)
Les Housever, one situation where GD was proven to solve
Les Housever, one situation where GD was proven to solve approximately F, problem
"Implicit bries of GD for wide 2-layers NNets" - Chizat and Bach, 2020.
Linear regime - Fz: problem adaptive to smoothness
Sometimes project fets
Non-luien dynamics - F. problem a adaptive la moothness
adaptive to low din proper Dreak curse of din. on these fet classes.



- · Limitation of kernel methods/linear models
 · Easture learning necessary to break the curse of

dimensionality

One "classical regime" example: GD futting underparametrized a single neuron with another neuron.

More realistic example where we can study feature learning with GD

$$\alpha \sim \text{Unif}(\xi \pm 13^d)$$

learning class of k-pointy fets

$$\mathcal{E}_{k} = \mathcal{E}_{k} \mathcal{E$$

Hardness result of learning parity fets with kernel methods

Prop: [Allen-Zhu et al., 2020] If for any fA & Ck $R_{lest}(\beta_*, \hat{\beta}_{\lambda}) \leqslant \frac{1}{9}$ (« d le) then we must have $M \geq \frac{3}{5} \binom{d}{k}$

Amle: 1) & (a) is a degree-ke polynomial, abready implied by previous result if kernel is an inir-product kernel then need no de samples here very elementary proof for any kernel
2) f _A (ri) only depend on a low-dimensional projection of dimension k —> expect F ₁ problem to be able to efficiently learn
Proof: [If time, probably not: very nice proof using only elementary algebra]
"Learning parities with neural networks" [Amit Daniely and Fran Malach, 2020]
With slightly different distribution + classification softing: $l(\hat{x}, y) - mon (1 - y \hat{y} = 0)$

+ 2 layers NNets with Relu activations

Thun: for any linear model $f(n) = \langle \psi(n), \hat{a} \rangle$ with $\psi(n) \in \mathbb{R}^N$ and $\|\hat{a}\|_2 \leq \mathbb{B}$, then there exists $\beta_A \in \mathcal{E}_k$ such that $\mathbb{R}_{\text{test}}(\beta_A, \hat{\beta}) \geq \frac{1}{2} - \frac{N}{2^k} \frac{\mathbb{B}}{2^k}$

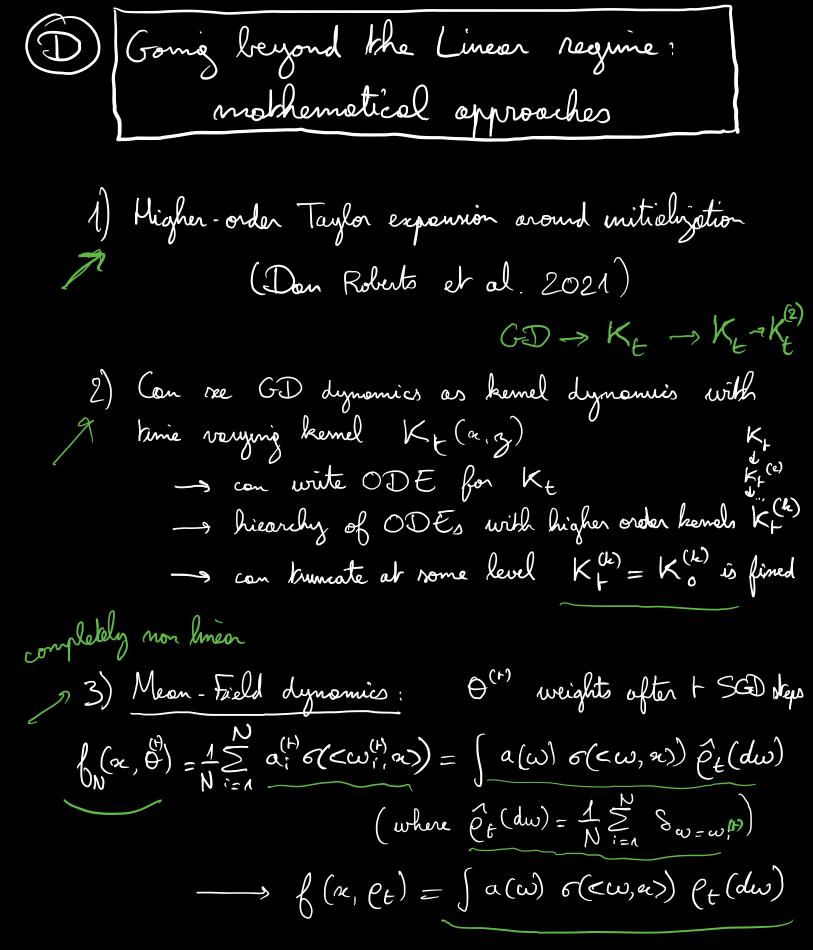
Thm: (informal) GD with some initialization and learning steps on population loss, for T steps with high probability, for any $6.1 \, \text{Ch}$ $R_{ket}(bA, \hat{k}^{(t)}) \lesssim \frac{h^8}{10} + \frac{Nk}{10} + \frac{k^2 \ln N}{10}$

Rmle: 1) le \times d²/₄, \times d⁴/₄, \times d²/₄

Then $\exists \beta_A \in \mathcal{C}_k \text{ much Halt}$ $\exists \beta_A \in \mathcal{C}_k \text{ much Halt}$

2) Still unsatisfactory: here $m=\infty$ (or very large) + artificial GD learning steps schedule

Proof idea: Initialization $\int_{0}^{\infty} \int_{0}^{\infty} (x, e^{(0)}) = \sum_{j=1}^{\infty} a_{j}^{(0)} G(\langle w_{j}^{(0)}, w_{j}^{(0)} \rangle) =$ 1 longe GD step $(1) \quad \int (\alpha, \theta^{(i)}) = \sum_{j=1}^{N} \alpha_j^{(i)} \quad \delta(\omega_j^{(i)}, \alpha)$ * learn good weights will karge correlation * show that if we fine wij and only known ag, con fit ba (2-5T) Following learning steps sufficiently small such bhat we are ni the lippear regime Sumery: (0) Initialize at a;0, co;0) 6D deps (1) One gradient step learn good cu;(1) (2-T) Eit second layer a (+) while w; (1) almost fined



PDE on le: evolution vi ble pace of measures

-> send paper: on Milliti-layer MF
Morro Mondelli generalizet error of
$\frac{b(x, 0^{t})}{b(x, 0^{t})} \longrightarrow 6^{t}$
MTK: FC multiloger NN everights NN(0, Id)
-> NTK h(ea,y) mer proof
1) learn only low d' poly on the sphere
2) F2-P _ not adapture
-> NTK: KRR with NT hernel

(1) $x \in \mathbb{R}^d$ $\alpha = U_3 + U_1 3$ $\alpha = U_3$ $\alpha = U_3$ $\alpha = U_3$ $\alpha = U_3 + U_1 3$ $\alpha = U_3 + U_1 3$