Artificial Neural Networks and Kernel Methods

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Introduction

Two competing methods in machine learning: **Neural Networks** and **Kernel Methods.**

Question: Did N.N. end the game ? Or is it a never-ending war ? Can these methods interact with each other ?

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Outline of the talk:

- ▷ **Introduction to Supervised Learning.**
- ▷ **Neural Networks and Neural Tangent Kernel.**
- ▷ **Theoretical and Practical Consequences.**
- ▷ **Extreme Learning and Regularized Kernel Methods.**
- ▷ **Kernel Method Generalization from the training set.**

Answer: Deep connections and interplay between Neural Networks and Kernel Methods.

Introduction to Supervised Learning

Abstraction and the Four Main Questions

Ideal Goal: to predict
e.g. : age of a person in a picture
$\downarrow$
Realistic Goal : train data
e.g. : "few" labelled pictures

Parameterized family
of functions : $(f_\theta)_{\theta \in \mathbb{R}^P}$

training part
$\longleftarrow$
$\longrightarrow$
optimization : θ^*

$\nearrow$
$\searrow$

Existence is not enough,
we want to find it.

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Generalization
You hope that the ideal goal is achieved

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You hope that the ideal goal is achieved

Does it learn ?	How does it learn ?	What does it learn ?	Is it useful ?
Training error	$(f_{\theta_t})_{t \geq 0}$	f_{θ^*}	Generalization error

General Setup: Regression, Predict $f^* : \mathbb{R}^{n_0} \longrightarrow \mathbb{R}^{n_{out}}$

Always assume $n_{out} = 1$, generalizable to $n_{out} > 1$.

Goal:

▷ *Ideal:* $\forall x, f_\theta(x) \sim f^*(x)$,

▷ *Proxy:* Functional Cost, e.g. M.S.E

$$\mathcal{C}(f) = \frac{1}{2} \int (f(x) - f^*(x))^2 \, d\mu(x),$$

▷ *Dataset:* $(x_i, y_i := f^*(x_i))_{i=1,\ldots,N}$,

▷ *Cost function* : Cost $\sim 0 \iff$ Goal achieved, e.g.

$$\mathcal{C}_N(f) = \frac{1}{2N} \sum_{i=1}^{N} (f(x_i) - y_i)^2 ,$$

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Model:

▷ *Parameterization:*

$$F : \theta \in \mathbb{R}^P \to \mathcal{F},$$

▷ *Parameters Cost Function:*

$$C = \mathcal{C}_N \circ F,$$

$\mathcal{C}_N$ is often convex, F can be not linear
$\Rightarrow$ the cost C might be non convex.

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Problem : Minimize C with an explicit algorithm: $\arg\min_\theta C(\theta)$.

Motivation: Two competing spaces of functions

Kernel methods

▷ $(\mathcal{H}, \langle\rangle_{\mathcal{H}})$ *Hilbert space* of real valued functions, evaluation on x continuous:

$$f(x) = \langle f, K_x \rangle_{\mathcal{H}} .$$

The kernel $K(x, y) = K_x(y)$ satisfies:

1. Symmetric $K(x, y) = K(y, x)$,
2. Matrices $(K(x_i, x_j))_{i,j}$ are positive semidefinite.

▷ Find f^* minimal norm in $\mathcal{H}$ such that $f(x_i) = y_i$ (or MSE+$\lambda \|f\|^2_{\mathcal{H}}$, $\lambda \searrow 0$).

▷ *Representer theorem*: f^* of the form

$$f_\theta(\cdot) = \sum_{i=1}^{N} \theta_i K(x_i, \cdot).$$

▷ Solution: $\theta^* = K(X, X)^{-1} Y$.

▷ **Ridgeless Kernel Regression:**

$$f_{\theta^*}(\cdot) = \sum_{i=1}^{N} \theta_i^* K(x_i, \cdot).$$

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Fully connected Artificial Neural Networks

▷ A parameterization of a *dense space of* functions:

$$f_\theta : \mathbb{R}^{n_0} \underset{A_1}{\longrightarrow} \mathbb{R}^{n_1} \underset{\sigma}{\longrightarrow} \mathbb{R}^{n_1} \underset{A_2}{\longrightarrow} \mathbb{R}^{n_2} \underset{\sigma}{\longrightarrow} \mathbb{R}^{n_2} \longrightarrow \ldots \mathbb{R}^{n_{L-1}} \underset{\sigma}{\longrightarrow} \mathbb{R}^{n_{L-1}} \underset{A_L}{\longrightarrow} \mathbb{R}^{n_{out}}$$

with:

1. $A_i : \mathbb{R}^{n_{i-1}} \to \mathbb{R}^{n_i}$ an affine function (the parameters),
2. $\boldsymbol{\sigma}$ the pointwise application of a non-linearity $\sigma : \mathbb{R} \to \mathbb{R}$.

▷ Find θ^* which minimizes the cost C.

▷ **Gradient descent.**

▷ Beliefs : Gradient descent will be stuck in good minimum.

Questions and answers

Are they so different?

1. Infinite Width Neural Network = Kernel Method
2. Infinite Width Neural Network with finite last hidden layer $\sim$ Kernel Method with Regularization

Can Kernel Method Theory give us a better insight on A.N.N.?

1. It allows us to answer the Four Main Questions for Infinite Width Neural Network: does it learn ? How does it learn ? What does it learn ? Does it generalize ?
2. Better insight into the architectural design of A.N.Ns.

Neural Networks and Neural Tangent Kernel

Main result: take away

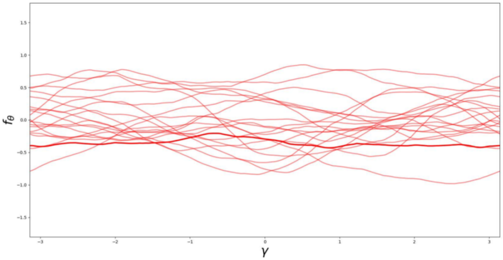
Theorem (Jacot, Gabriel, Hongler, NeuRIPS 2018)

Gradient Descent Learning for Infinite Width Limit Neural Networks

$\|$

Kernel Method for the Neural Tangent Kernel (N.T.K.)

Illustration



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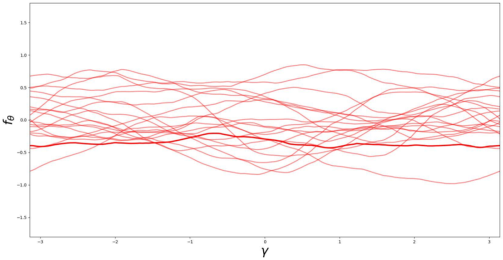
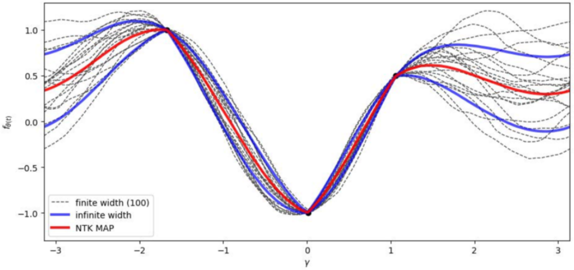
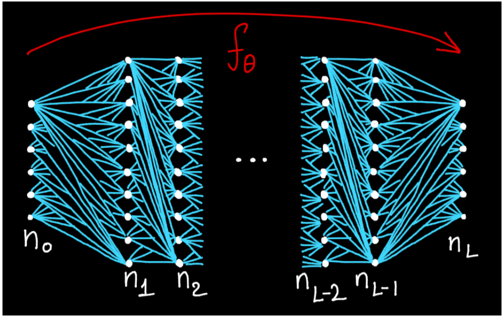




Setup: Fully Connected Neural Networks

A Fully Connected Neural Network:

- **Non linearity:** $\sigma : \mathbb{R} \to \mathbb{R}$, e.g. $ReLU(x) = \max(0, x)$. (Lipschitz, twice differentiable nonlinearity function for our theorem),
- **Number of hidden layers:** $L - 1$,
- **Sizes of the layers:** $n_{in} = n_0, n_1, \ldots, n_{L-1}, n_L = n_{out} = 1$.



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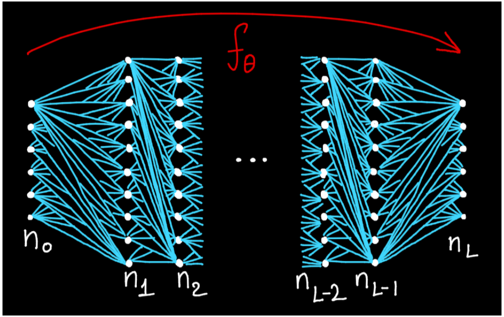

$$f_\theta^{(L)} : \mathbb{R}^{n_0} \xrightarrow[x \mapsto \frac{1}{\sqrt{n_0}} W^{(0)} x + \beta b^{(0)}]{} \mathbb{R}^{n_1} \xrightarrow{\sigma} \mathbb{R}^{n_1} \xrightarrow[x \mapsto \frac{1}{\sqrt{n_1}} W^{(1)} x + \beta b^{(1)}]{} \ldots \xrightarrow{\sigma} \mathbb{R}^{n_{L-1}} \xrightarrow[x \mapsto \frac{1}{\sqrt{n_{L-1}}} W^{(L-1)} x + \beta b^{(L-1)}]{} \mathbb{R}$$

▷Ptw. application of σ,

▷The parameters : $(\theta_p)_{p \in [P]} = \left(W^{(0)}, b^{(0)}, \ldots, W^{(L-1)}, b^{(L-1)}\right)$.

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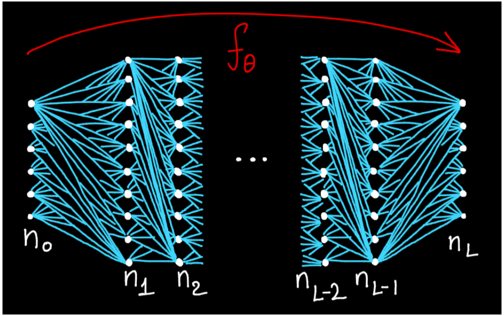

Activations $\alpha^{(\ell)}$. Preactivations $\tilde{\alpha}^{(\ell)}$. Output function $f_\theta(x) = \tilde{\alpha}^{(L)}(x)$

$$\tilde{\alpha}^{(\ell+1)}(x) = \frac{1}{\sqrt{n_\ell}} W^{(\ell)} \alpha^{(\ell)}(x) + \beta b^{(\ell)},$$

$$\alpha^{(\ell+1)}(x) = \sigma\left(\tilde{\alpha}^{(\ell+1)}(x)\right),$$

with pointwise application of σ.

Setup: Algorithm, the gradient descent

We implement a *first-order algorithm* and we want the cost to decrease:

$$\theta \to \theta + d\theta \quad \Rightarrow \quad C(\theta) \to C(\theta) + \langle \nabla C(\theta), d\theta \rangle$$

$$\hookrightarrow \quad d\theta \propto -\nabla C(\theta)$$

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Cost

$C = \mathcal{C}_N \circ F$, i.e.

$$C(\theta) = \frac{1}{2N} \sum_{i=1}^{N} (f_\theta(x_i) - y_i)^2$$

Algorithm

Gradient Descent:

$$d\theta = -\nabla C(\theta) dt,$$

Gradient Flow:

$$\partial_t \theta_t = -\nabla C(\theta_t)$$

Initialization

If $(\theta_p)_{p=1,\ldots P} = 0$, the gradient descent gets stuck.
Idea [LeCun/He init.]

$$(\theta_p)_{p=1,\ldots P} \sim \mathcal{N}(0,1) \text{ i.i.d.}$$

New Object: The N.T.K.

How can we describe the training of N.N?

Study the dynamics of f_{θ_t} and not of θ_t.

How?

Using a new kernel

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The Neural Tangent Kernel

$$\Theta^{(L)}(x_1, x_2) = \sum_{p=1}^{P} \frac{\partial f_\theta}{\partial \theta_p}(x_1) \frac{\partial f_\theta}{\partial \theta_p}(x_2) = \langle \nabla_\theta f_\theta(x_1), \nabla_\theta f_\theta(x_2) \rangle .$$

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It is *random* at initialization and *evolves with time.*

NTK and the learning dynamics.

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Theorem (Jacot, Gabriel, Hongler 18)

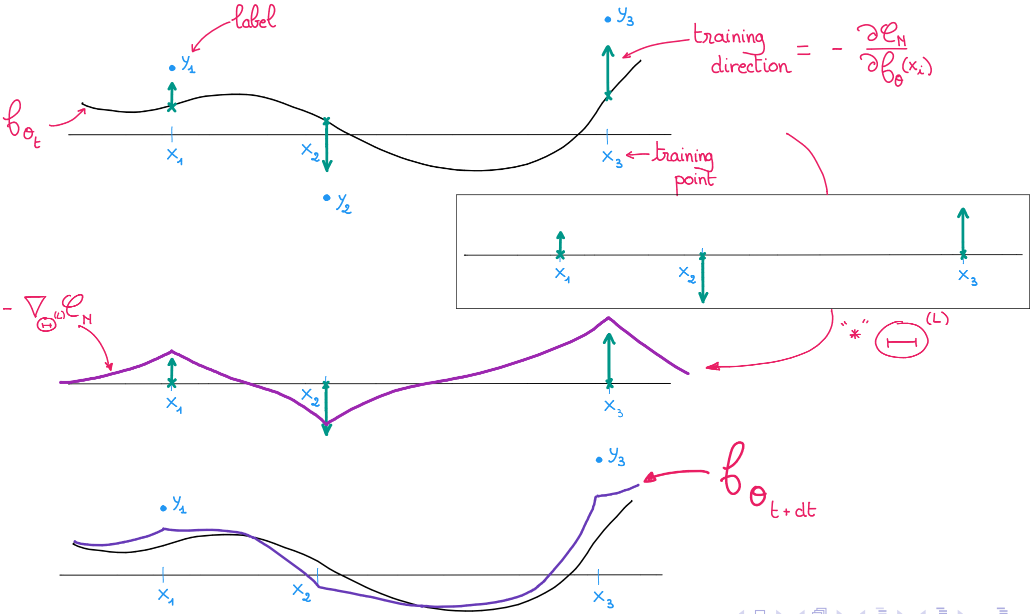
Consider a Fully Connected Neural Network with $L-1$ hidden layers of width $n_1, \ldots n_{L-1}$: $f_\theta : \mathbb{R}^{n_{in}} \to \mathbb{R}$. During Gradient Descent:

$$\partial_t f_{\theta_t} = -\nabla_{\Theta_t^{(L)}} \mathcal{C}_N,$$

where

$$\nabla_{\Theta_t^{(L)}} \mathcal{C}_N(x) = \sum_{i=1}^{N} \Theta_t^{(L)}(x, x_i) \frac{\partial \mathcal{C}_N}{\partial f_{\theta_t}(x_i)}.$$

Illustration: Dynamics



Proof: Dynamics

Recall that $C = \mathcal{C}_N \circ F$, with $\mathcal{C}_N(f) = c(f(x_1), \ldots, f(x_N))$.

- Parameter Space: $d\theta_p = -\frac{\partial C}{\partial \theta_p} dt = -\sum_{i=1}^{N} \frac{\partial f_\theta}{\partial \theta_p}(x_i) \frac{\partial \mathcal{C}_N}{\partial y_i} dt$.

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- Function Space:

$$f_\theta(x) \to f_{\theta + d\theta}(x) \quad \sim \quad f_\theta(x) + \sum_{p=1}^{P} d\theta_p \frac{\partial f_\theta}{\partial \theta_p}(x)$$

$$f_\theta(x) - \sum_{i=1}^{N} \left[\sum_{p=1}^{P} \frac{\partial f_\theta}{\partial \theta_p}(x) \frac{\partial f_\theta}{\partial \theta_p}(x_i) \right] \frac{\partial \mathcal{C}_N}{\partial f(x_i)} dt.$$

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\partial_t f_{\theta_t}(x) = -\sum_{i=1}^{N} \Theta^{(L)}(x, x_i) \frac{\partial \mathcal{C}_N}{\partial y_i} dt = -\nabla_{\Theta^{(L)}} \mathcal{C}_N.
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Main Theorem

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Consider a Fully Connected Neural Network with $L-1$ hidden layers of width $n_1, \ldots n_{L-1}$: $f_\theta : \mathbb{R}^{n_{in}} \to \mathbb{R}$.

1. *During Gradient Descent:*
$$\partial_t f_{\theta_t} = -\nabla_{\Theta_t^{(L)}} \mathcal{C}_N.$$
2. *When $n_1, \ldots, n_{L-1} \to \infty$ sequentially:*
   - *At initialization, $f_{\theta_0} \sim \mathcal{N}(0, \Sigma^{(L)})$ [Neal 96, de G. Matthews and al 17,18].*
   - *The NTK:*
     - *At initialization, becomes **deterministic**:*
$$\Theta_{t=0}^{(L)} \longrightarrow \Theta_{t=0,\infty}^{(L)}.$$
     - *Becomes **fixed during training**: uniformly on $t \leq T$*
$$\left|\Theta_t^{(L)}(x_1, x_2) - \Theta_{t=0,\infty}^{(L)}(x_1, x_2)\right| \to 0.$$

Limiting dynamics

The limiting trajectory is

$$\partial_t f_{\theta_t} = -\nabla_{\Theta_\infty^{(L)}} \mathcal{C},$$

which **converges to a global minimum** if the cost functional $\mathcal{C}$ is convex and lower bounded and $\Theta_\infty^{(L)}$ is positive definite.

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Theorem (Jacot, Gabriel, Hongler 18)

Assume that the data $x_1, \dots, x_N$ lie on a sphere:
$\Theta_\infty^{(L)}$ is definite positive for any input dimension n_{in} i.i.f. σ is a non polynomial function.

General Idea

Main Idea: break down an FCNN of size $L+1$ as a FCNN of size L followed by the pointwize application of σ and an affine map.

$$f_\theta^{(L+1)} : \mathbb{R}^{n_0} \xrightarrow{f_\theta^{(L)}} \mathbb{R}^{n_L} \xrightarrow{\sigma} \mathbb{R}^{n_L} \xrightarrow{A_L} \mathbb{R}$$

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This intuition holds during:

- **inference:** i.e. when you evaluate $f_\theta^{(L+1)}$,
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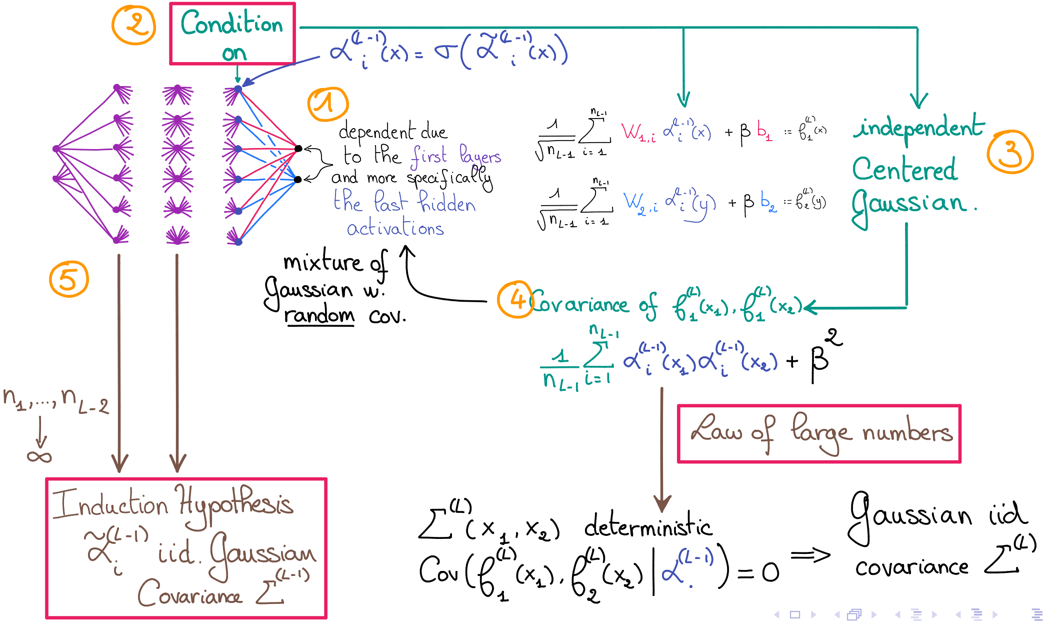
Main Tools:

- Induction on the number of layers L,
- Law of large number,
- CLT,
- Generalized Grönwall's inequalities.

Proof: $f_{\theta_L} \sim \mathcal{N}$



Proof: $\Theta^{(L)}_{t,n} \to \Theta^{(L)}_{\infty}$, the inner parameters

$$f_\theta^{(L+1)}(x) = \frac{1}{\sqrt{n_L}} \sum_{k=1}^{n_L} W^{(L)}_{1,k}\, \sigma\left(f_\theta^{(L)}(x)\right) + \beta\, b_1^{(L)}$$

$$\Theta^{(L+1)}_{\text{inner}}(x_1,x_2) = \sum_{\theta_p \in \text{ANN}^{(L)}} \frac{\partial}{\partial \theta_p} f_\theta^{(L+1)}(x_1)\, \frac{\partial}{\partial \theta_p} f_\theta^{(L+1)}(x_2)$$

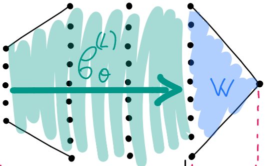
$$\frac{1}{\sqrt{n_L}} \sum_{k=1}^{n_L} W^{(L)}_{1,k}\, \dot\sigma\left(f_\theta^{(L)}(x_1)\right) \frac{\partial}{\partial \theta_p} f_\theta^{(L)}(x_1) \qquad \frac{1}{\sqrt{n_L}} \sum_{k=1}^{n_L} W^{(L)}_{1,k}\, \dot\sigma\left(f_\theta^{(L)}(x_2)\right) \frac{\partial}{\partial \theta_p} f_\theta^{(L)}(x_2)$$

$$\Theta^{(L+1)}_{\text{inner}}(x_1,x_2) = \frac{1}{n_L} \sum_{k,k'=1}^{n_L} W^{(L)}_{1,k} W^{(L)}_{1,k'}\, \dot\sigma\left(f_\theta^{(L)}(x_1)\right) \dot\sigma\left(f_\theta^{(L)}(x_2)\right) \Theta^{(L)}_{k,k'}(x_1,x_2)$$

Law of Large Numbers ⟸ Induction Hyp. $n_1, \dots, n_{L-1} \to \infty$

$\Theta^{(L+1)}_{\text{inner},\infty}(x_1,x_2)$ deterministic $\qquad \delta_{k,k'}\, \Theta^{(L)}_\infty(x_1,x_2)$

Sketch of proof: $\Theta_t^{(L)} \to \Theta_\infty^{(L)}$



(1) train the first layers with a time dep cost: $C_N\left(\frac{1}{\sqrt{n_L}}\sum_{k=1}^{n_L} W_k^{(L)}(t)\,\sigma(f_{\theta_t,k}^{(L)})+\beta b_1\right)$

train the last layer (3)

Which dynamics $n_1,\dots,n_{L-1}\to\infty$? Induction Hyp (2)

$$\partial_t f_\theta^{(L)} = -\frac{1}{\sqrt{n_L}}\,\Theta_\infty^{(L)}\otimes Id\,(\dots)$$ $W_k^{(L)}$

$$d\,W_k(t) = -\frac{1}{\sqrt{n_L}}\sum_{i=1}^{N}\sigma(f_{\theta_t}^{(L)}(x_i))\,\frac{\partial C_N}{\partial y_i}\,dt$$

(4) $f_\theta^{(L)} \xrightarrow{1/\sqrt{n_L}} W_k^{(L)}(t)$

$W_k^{(L)}(t) \xrightarrow{1/\sqrt{n_L}} \Theta_p$ $\Longrightarrow$ Grönwall

$\Theta_p \to f_\theta^{(L)}$: NTK dynamics

W, $f_\theta^{(L)}$ vary at rate $1/\sqrt{n_L}$ $\Longrightarrow$ idem pour NTK

Generalization: multiple output

Generalize to multi-dimensional output:

- $\Theta^{(L)}_{k,k'}(x,x') = \sum_{p=1,\dots,P} \frac{\partial f_{\theta,k}}{\partial \theta_p}(x)\frac{\partial f_{\theta,k'}}{\partial \theta_p}(x')$.
- $\partial_t f_{\theta_t} = -\nabla_{\Theta^{(L)}_t} \mathcal{C}_N$ with $\left(\nabla_{\Theta^{(L)}_t} \mathcal{C}_N\right)_k = \sum_{i=1}^{N} \sum_{k'=1}^{n_{out}} \Theta^{(L)}_{t,k,k'}(\cdot, x_i) \frac{\partial \mathcal{C}_N}{\partial f_{\theta_t,k'}(x_i)}$.

Generalization: multiple output

Generalize to multi-dimensional output:

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Main Features of the Multiple Output Setting:

- At initialization, $(f_{\theta_0,k})_{k=1}^{n_{out}}$ are **i.i.d.**
- The limiting NTK is **diagonal:**

$$\left(\Theta^{(L)}_\infty\right)_{k,k'}(x,x') = \left(\Theta^{(L)}_\infty(x,x')\right)\delta_{k,k'}.$$

- The functions $(f_{\theta,k})_{k=1}^{n_{out}}$ **evolve independently.**

Other Generalizations

Since then (May 2018), many generalizations:

- Finite time step, large but finite width, infinite time horizon for M.S.E **[Du S. for 2 layers ReLU $\sim$ NTK (2018)], [Allen-Zhu et al. (2018)], [many papers of Arora S., Du S. and al (2019)]**
- Lazy training: **[Chizat-Bach (2018)]**, **[Lee, Xiao and al. (2019)]**
- Taylorised learning **[Huang, Yau (2019)]** : Neural Tangent Hierarchy, N^3 width enough. Fluctuations($\Theta^{(L)}_{t=0}$)$\sim P^{-\frac{1}{4}}$, Fluctuations($\Theta^{(L)}_t - \Theta^{(L)}_{t=0}$)$\sim P^{-\frac{1}{2}}$. **[Bai and al. (2020)]**
- Other architectures at initialization: Tensor Programs of Greg Yang (2019)
- Other optimization algorithm:
  - Momentum **[Lee, Xiao and al. (2019)]**
  - Natural gradient **[Rudner, Teh, Wenzel, Gal (2019)]**

Theoretical and Practical Consequence on ANN Learning

Reminder

The dynamics of f_{θ_t} during training is given by:

Finite size		Randomness	Large limit
	$\nearrow$	Random initial kernel $\Theta^{(L)}_{t=0}$	Deterministic
$\partial_t f_{\theta_t} = -\nabla_{\Theta^{(L)}_t} \mathcal{C}_N,$	$\longrightarrow$	Random evolution of $\Theta^{(L)}_t$	Constant in time
f_{θ_0}	$\searrow$	Random initial function f_{θ_0}	$f_{\theta_0} \sim \mathcal{N}\left(0, \Sigma^{(L)}\right)$

Answer to the Four Questions: how and what?

General setting

- Dynamics:

$$\partial_t f_{\theta_t}(x) = -\sum_{x_i} \Theta^{(L)}(x, x_i) \frac{\partial \mathcal{C}_N}{\partial f_{\theta_t}(x_i)}$$

  Hence: $f_{\theta_t} = f_0 + \sum \vartheta_{i,t} \Theta^{(L)}(x, x_i)$.
- Final function:
  $f_0 +$ Kernel method for $\mathcal{C}_N(\cdot + f_0)$

Answer to the Four Questions: how and what?

General setting

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$$\partial_t f_{\theta_t}(x) = -\sum_{x_i} \Theta^{(L)}(x, x_i) \frac{\partial \mathcal{C}_N}{\partial f_{\theta_t}(x_i)}$$

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- Final function: $f_0 +$ Kernel method for $\mathcal{C}_N(\cdot + f_0)$

MSE

- For MSE, $\frac{\partial \mathcal{C}_N}{\partial f_{\theta_t}(x_i)} = f_{\theta_t}(x_i) - y_i$: linear differential equation.
- On training points, the Gram matrix yields the speed of convergence.
- The function is Gaussian during training.
- Final function: $f_{\theta_\infty} = f_0 + \mathrm{KR}_{\lambda=0,(X,Y)}(f^* - f_0)$ or

$$f_{\theta_\infty} = \mathrm{KR}_{\lambda=0,(X,Y)}\left(f^*\right) + \epsilon,$$

  with **noise error term** $\epsilon = f_0 - \mathrm{KR}_{\lambda=0,(X,Y)}(f_0)$. [Zhang, Xu and al (2019)]

Answer to the Four Questions: train error and generalization?

- **Training:**

For MSE loss: training loss $= 0$. In general minimun error loss attained.

- **Generalization:**

Very large FCNN should generalize as RKHS methods: Rademacher bound should yield bounds of the form $\sqrt{\frac{Y\Theta^{-1}Y}{N}}$ for bounded Lip. cost. **[Arora, Du and al 2019 - 2 Layer ReLu and bounded Lip. cost function]**

Consequences: Training of large depth networks

Order-Chaos during inference [Daniely and al. 2016] [S.S. Schoenholz and al. 2017] [Hayou, Doucet, Rousseau 2019]
Depending on the variance of the initialisation as $L \to \infty$: $\Sigma^{(L)} \to C$ (order) or $\Sigma^{(L)} \to C_1 + C_2 \delta_{x=y}$ (chaos)

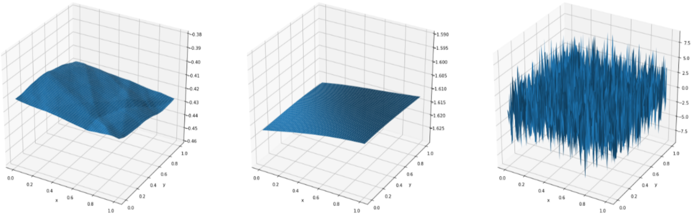

Figure: From “On the Impact of the Activation Function on Deep Neural Networks Training” [Hayou and al]

Consequences: Training of large depth networks

Freeze-Chaos during training [Jacot, Gabriel, Hongler 2019] [Agarwal, Awasthi, Kale 2020]
Depending on the variance of the initialisation:

- $\Theta^{(L)} \to C$ (order), the bias are two important, difficult to train.
- $\Theta^{(L)} \sim C_L \delta_{x=y}$ (chaos), easier to train, but generalization not good.

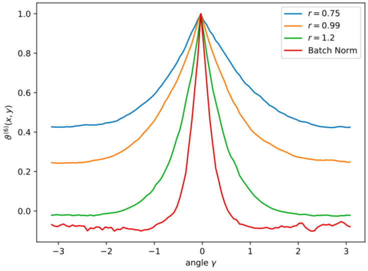

Figure: From "Order and Chaos: NTK views on DNN Normalization, Checkerboard and Boundary Artifacts" [A. Jacot, F. Gabriel, F. Ged, C. Hongler]

Consequences:Generalization

Function loss is convex : *noise in the predictor is bad.*

$$\mathbb{E}\left[\int (f_{\theta_\infty}(x) - f^*(x))^2 \, d\mu(x)\right] = \underbrace{\int (\mathbb{E}(f_{\theta_\infty}(x)) - f^*(x))^2 \, d\mu(x)}_{\text{Bias}} + \underbrace{\int \mathbb{V}\text{ar}\,[f_{\theta_\infty}(x)] \, d\mu(x)}_{\text{Variance}}$$

- The noise due to f_{θ_0} can be suppressed: train $f_\theta - f_{\theta_0}$ instead of f_θ
  - same dynamics + initialization $= 0 \to$ Kernel method
- ["Scaling description of generalization with number of parameters in deep learning", Geiger, Jacot, Spigler, **Gabriel**, Sagun, d'Ascoli, Biroli, Hongler, Wyart]
  Still noise due to fluctuations($\Theta^{(L)}_{t=0}$)$\sim P^{-\frac{1}{4}}$ and fluctuations($\Theta^{(L)}_t - \Theta^{(L)}_{t=0}$)$\sim P^{-\frac{1}{2}}$
  - Fluctuations of $f_{\theta_\infty}(x) \sim P^{-\frac{1}{4}}$, and Variance $\sim P^{-\frac{1}{2}}$,
  - If bias is constant in overparameterized regime:

$$\text{Generalization error} \sim \text{Error}_{P=\infty} + P^{-\frac{1}{2}}.$$

Double curve descent phenomenon

Extreme Learning and Regularized Kernel Method

Extreme Learning

Extreme Learning $=$ Learning the last layer's parameters.

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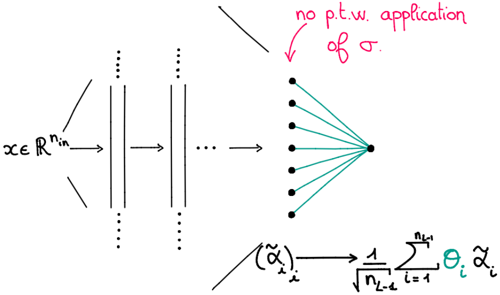


▷ To simplify, we consider no bias (i.e. no additive parameter) for the last layer, and we assume that there is no pointwise application of the non-linearity at the last hidden layer.
▷ We assume that all hidden layers, except the last one, are infinite $\Longrightarrow f_i^{(L-1)}$ are i.i.d. $\mathcal{N}\left(0, \Sigma^{(L-1)}\right)$.
▷ We train only the last hidden layer, with a ℓ_2-norm penalization on $\boldsymbol{\theta}$.

Result : This is close to a Kernel Method with kernel $\Sigma^{(L-1)}$ but with a **larger regularisation.**

Implicit Regularization of Finite Sampling of Features

Rahimi & Recht's Random Features

$$f_{\boldsymbol{\theta}} : \mathbb{R}^{n_{in}} \xrightarrow{f} \mathbb{R}^{P} \xrightarrow[x \to \frac{1}{\sqrt{P}} \boldsymbol{\theta} x]{} \mathbb{R}$$

- f is an infinite neural network at initialization (recall: no pointwise application of σ for the output layer) **in particular,** $f = (f_j)_{j=1}^{P}$ **i.i.d. G.P.** $\mathcal{N}(0, K)$.
- The parameters are $\boldsymbol{\theta} \in \mathbb{R}^{P}$, and we consider N data points $(x_i, y_i)_{i=1}^{N}$.
- Optimization with $\frac{\lambda}{N} > 0$ penalization on the ℓ_2-norm of $\boldsymbol{\theta}$.

$$\min_{\boldsymbol{\theta}} \frac{1}{N} \sum_{i=1}^{N} \left(f_{\boldsymbol{\theta}}(x_i) - y_i \right)^2 + \frac{\lambda}{N} \|\boldsymbol{\theta}\|^2$$

- Closed Formulae: With $F_{ij} = \frac{1}{\sqrt{P}} f_j(x_i)$, optimal parameter: $\hat{\theta} = \left(F^T F + \lambda I_P \right)^{-1} F^T y$ leads to prediction: $\hat{y} = \underbrace{F \left(F^T F + \lambda I_P \right)^{-1} F^T}_{A_\lambda} y$ and optimal predictor:

$$\hat{f}_{\lambda}^{(RF)}(x) = \frac{1}{\sqrt{P}} \sum_{j=1}^{P} \hat{\theta}_j f_j(x).$$

Large number of features

$$\hat{y} = \underbrace{F\left(F^T F + \lambda I_P\right)^{-1} F^T}_{A_\lambda} y$$

But:

$$F\left(F^T F + \lambda I_P\right)^{-1} F^T = FF^T\left(FF^T + \lambda I_P\right)^{-1}$$

with

$$\left(FF^T\right)_{i,j} = \frac{1}{P}\sum_k f_k(x_i) f_k(x_j) \underset{P\to\infty}{\longrightarrow} K(x_i, x_j)$$

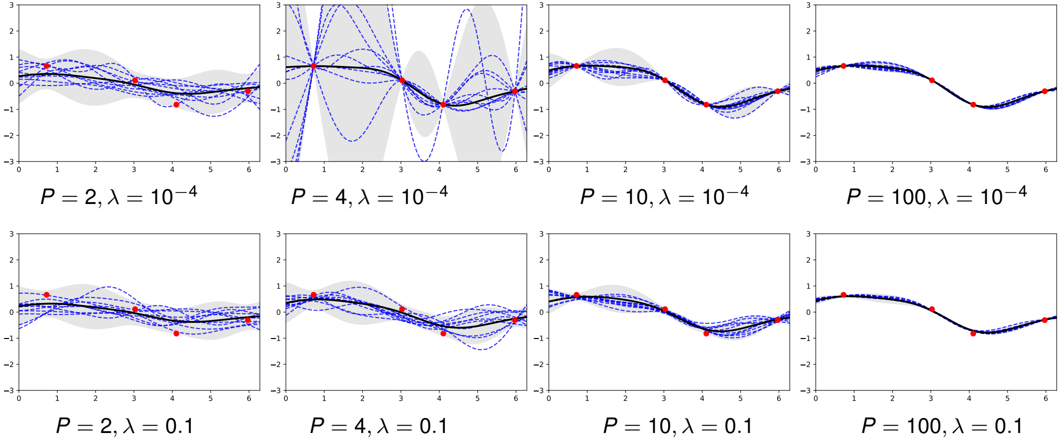
Thus:

$$\hat{y} \to K(X,X)\left[K(X,X) + \lambda I_N\right]^{-1} y$$

and the predictor converge to the K Kernel predictor with ridge λ:

$$\hat{f}_\lambda^{(RF)}(x) \to \hat{f}_\lambda^{(K)}(x) := K(x,X)\left[K(X,X) + \lambda I_N\right]^{-1} y.$$

R.F. Predictor



$P = 2, \lambda = 10^{-4}$ $P = 4, \lambda = 10^{-4}$ $P = 10, \lambda = 10^{-4}$ $P = 100, \lambda = 10^{-4}$

$P = 2, \lambda = 0.1$ $P = 4, \lambda = 0.1$ $P = 10, \lambda = 0.1$ $P = 100, \lambda = 0.1$

Finite number of features

$$\hat{y} = \underbrace{F\left(F^T F + \lambda I_P\right)^{-1} F^T}_{A_\lambda} y, \qquad \mathbb{E}\left[\hat{f}_\lambda^{(RF)}(x)\right] = \Sigma^{(L)}(x,X)\Sigma^{(L)}(X,X)^{-1}\mathbb{E}\left[A_\lambda\right] y$$

▷ The matrix A_λ can be studied using the **Stieljes transform**: $\frac{1}{P}\mathrm{Tr}\left[\left(F^T F + \lambda I_P\right)^{-1}\right]$

▷ The matrix F as a special structure: its columns are i.i.d. and Gaussian with cov $\frac{1}{P}K$:

$$F \sim \frac{1}{\sqrt{P}} K^{1/2} W^T$$

where W is a $P \times N$ random matrices with entries i.i.d. standard Gaussian.

▷ For the matrix $F^T F$:

$$F^T F \sim \frac{1}{P} W K W^T,$$

whose Stieljes transform can be studied like $K\left(\frac{1}{P} W^T W\right)$: product of a **Wishart Matrix** and a **deterministic matrix, well studied in free probability.**

Main result

Theorem (A. Jacot, B. Şimşek, F. Spadaro, C. Hongler, F. Gabriel, ICML 2020)

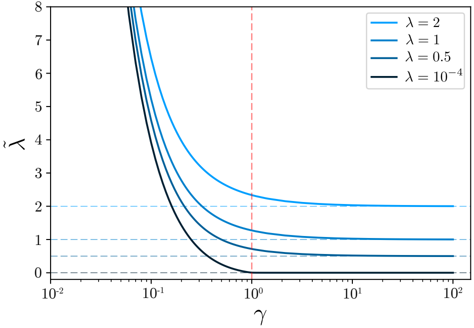
Even for $P < \infty$, $\mathbb{E}\left[\hat{f}_{\lambda}^{(RF)}(x)\right]$ is close to the Kernel predictor $\hat{f}_{\tilde{\lambda}}^{(K)}$ with a larger "effective ridge" $\tilde{\lambda}(\gamma, \lambda) > \lambda$ which is the unique solution of

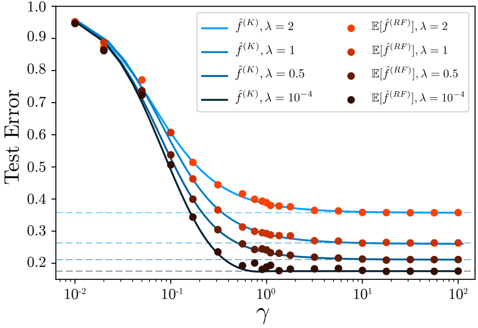
$$\tilde{\lambda} = \lambda + \frac{\tilde{\lambda}}{\gamma} \frac{1}{N} \mathrm{Tr}\left(K(X, X) \left(K(X, X) + \tilde{\lambda} \right)^{-1} \right),$$

where $K(X, X)$ is the Gram matrix of K.

*It is the **implicit regularization effect** of finite random features sampling.*

Effective Ridge and Test Error



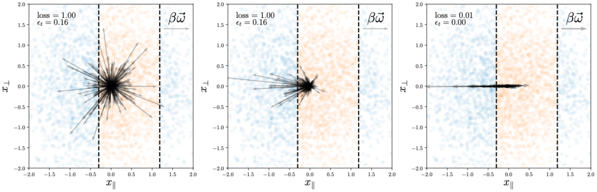


Kernel Method Generalization from the training set

Experiments on Structured Data and Finite N.N.

Recent pre-print of J. Paccolata, L. Petrinia, M. Geigera, K. Tylooa, and M. Wyart:
Setting: Classification with hinge Loss $c(y, y^*) = (1 - yy^*)^+$, shallow network, labels only depends on the first coordinate (stripe model), parameters initialized very small (feature learning regime).
Three phases during learning:

1. **Compressing Regime:** Parameters evolve independently and tend to align with the informative subspace.

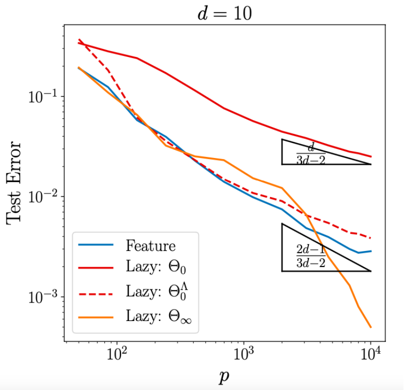


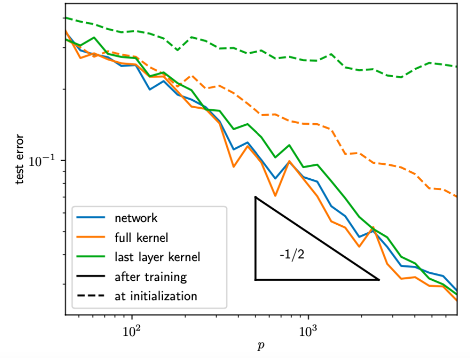
2. **Fitting regime:** when a fraction of constraints are satified, the N.N. tries to fit the labels but the parameters still evolve within the informative subspace.
3. **Over-fitting regime.**

Question: Is the N.T.K. theory no more interesting ?

Final NTK v.s. Neural Network

Answer: No, the kernel dynamics is still true but with an evolving kernel and in their experiment the NTK at the end of training is as good as the Neural Network !





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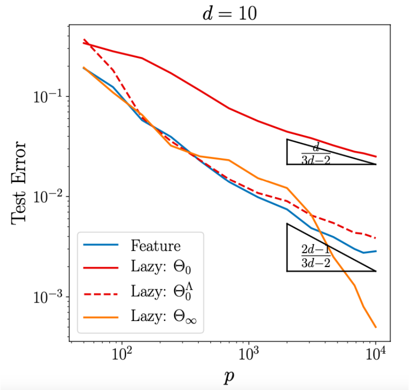
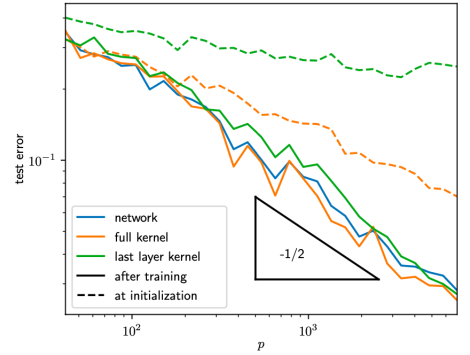
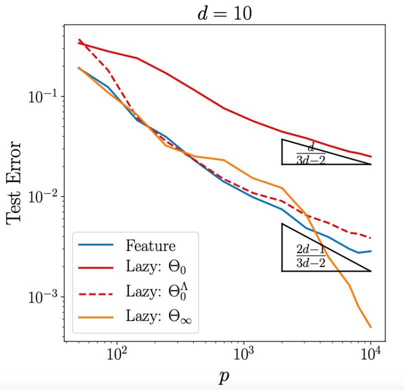


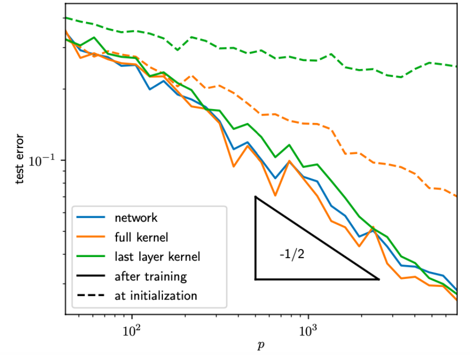


Question (Open): How does the N.T.K. improves ? How does the Neural Network "knows" that the kernel needs to evolve, based only on the training points ?

Final NTK v.s. Neural Network

Answer: No, the kernel dynamics is still true but with an evolving kernel and in their experiment the NTK at the end of training is as good as the Neural Network !





Question: Can we estimate the generalization error of a kernel method, based only on the training points ?

K.A.R.E. : the Kernel Alignement Risk Estimator

Consider a Kernel Method for

▹ Random i.i.d. training points $x_i \sim \mathcal{D}$ in a compact domain Ω

▹ Training labels $y_i^* = f^*(x_i) + \epsilon e_i$ with $e_i \sim \mathcal{N}(0,1)$

▹ Minimizing $\frac{1}{N}\sum_{i=1}^{N}\left(f(x_i) - y_i^*\right)^2 + \lambda \|f\|_{\mathcal{H}}^2$, i.e.

$$\hat{f}_\lambda(x) = K(x,X)\left[K(X,X) + \lambda I_N\right]^{-1} Y^*$$

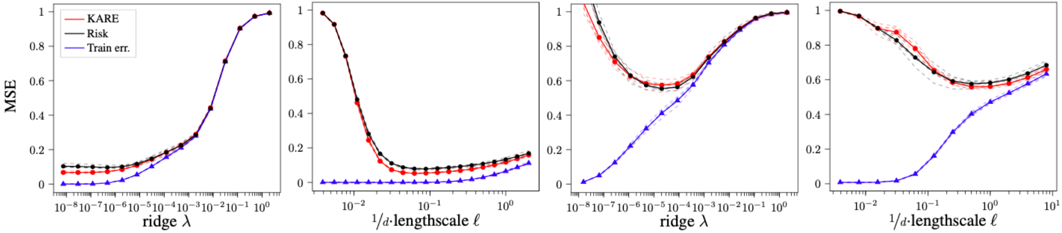
Fact (A. Jacot, B. Şimşek, F. Spadaro, C. Hongler, F. Gabriel, 2020)

We propose the following estimator of the Risk of the Kernel predictor $\hat{f}_\lambda$ with ridge λ :

$$\mathbb{E}_{x_1,\ldots,x_n,x\sim\mathcal{D}}\left[\left(\hat{f}_\lambda(x) - f^*(x)\right)^2\right] + \epsilon^2 \approx \frac{\frac{1}{N} Y^* \left[\frac{1}{N}K(X,X) + \lambda I_N\right]^{-2} Y^*}{\left(\frac{1}{N}\mathrm{Tr}\left[\left(\frac{1}{N}K(X,X) + \lambda I_N\right)^{-1}\right]\right)^2} = K.A.R.E.$$

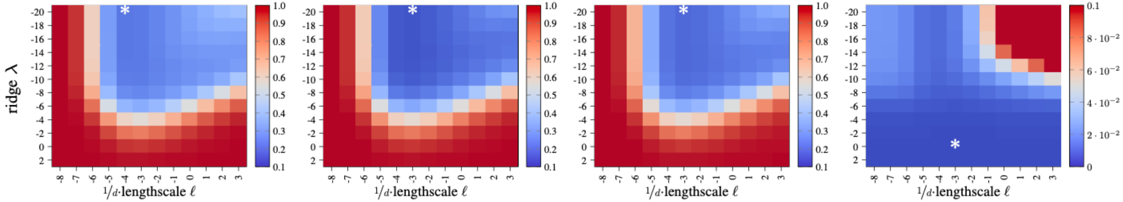
A theorem if only the second moments of the observations matters.

Experiments on Real Data



(a) MNIST, $\ell = d$ (b) MNIST, $\lambda = 10^{-5}$ (c) Higgs, $\ell = d$ (d) Higgs, $\lambda = 10^{-4}$

Hyperparameter selection with K.A.R.E.



(a) Risk (b) KARE Predictions (c) Cross Val. Predictions (d) Log-likelihood Estim.

Conclusion

To Wrap Up the Presentation

Recursive structure of A.N.N. $\Longrightarrow$ attractive properties. The training of A.N.N. using Gradient Descent with Random Initialization explained using the Neural Tangent Kernel. In the infinite width limit,

- the N.T.K. is **deterministic** and **constant during training,**
- the function follows a **Kernel Gradient Descent** with fixed kernel,
- the N.T.K. is > 0 and the **limiting dynamics converges to a global minimum,**
- the final function is of the form **Noise + Kernel Method**, and by a slight change on the definition of ANN, it becomes a **deterministic Kernel Method**.

In the finit width case:

- Fuctuations of the N.T.K. at initialization are the most important **and decrease with** P**: generalization error decreases as** $P^{-\frac{1}{2}}$ $\rightarrow$ **double curve descent is expected.**
- Last hidden layer finite followed by linear map, last parameters learned with ℓ^2 penalty with ridge λ: again **close to a Kernel Method with an other so-called "effective" ridge** $\tilde{\lambda} \geq \lambda$**.**

Kernel Method:

- Propose a **new estimator** for the **risk** for Kernel Methods: the **KARE**.

Thank you !

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