Mean Field Theory and Tangent Kernel Theory of Neural Networks

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Deep learning applications

- Computer vision (autonomous vehicles).
- Generative modeling (WaveNet for generating speech).
- Reinforcement learning (Go playing).
Mathematical challenges/mysteries

- Optimization → Non-convexity.
- Generalization → Overparameterization.
Agenda

1. Mean field theory

2. Tangent kernel theory

3. Transitions between mean field and tangent kernel regime
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1. Mean field theory

2. Tangent kernel theory

3. Transitions between mean field and tangent kernel regime
Two-layers neural networks

Figure: $\theta_i = (a_i, w_i)$. 
Two-layers neural networks

- Parameters: \( \theta = (\theta_1, \ldots, \theta_N) \in \mathbb{R}^{N \times D}. \)

- Prediction function:

\[
f(x; \theta) = \frac{1}{N} \sum_{i=1}^{N} \sigma(x; \theta_i) = \frac{1}{N} \sum_{i=1}^{N} a_i \sigma(\langle w_i, x \rangle).
\]

- Risk function:

\[
R_N(\theta) = \mathbb{E}_{x,y} \left[ \ell(y, \frac{1}{N} \sum_{i=1}^{N} \sigma(x; \theta_i)) \right].
\]

- Gradient flow for \( R_N \):

\[
\frac{d}{dt} \theta_t = -N \xi(t) \nabla_{\theta_t} R_N(\theta_t).
\]

- Difficulty: non-convexity with local minimizers!
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- **Gradient flow for $R_N$:**

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- Gradient flow for $R_N$:

$$\frac{d}{dt} \theta^t_i = -N \xi(t) \nabla_{\theta_i} R_N(\theta^t).$$  \hspace{2cm} (GF)

- Difficulty: non-convexity with local minimizers!
Landscape analysis?

\[ R_N(\theta) = \mathbb{E}_{x,y} \left[ \left( y - \frac{1}{N} \sum_{j=1}^{N} \sigma_*(x; \theta_j) \right)^2 \right]. \]

- [Kawaguchi, 2016], [Freeman, Bruna, 2016]: linear network has no spurious local min.
- [Soltanolkotabi, Javanmard, Lee, 2017]: Quadratic two-layers NN has no spurious local min.
- [Zhong, Song, Jain, Bartlett, Dhillon, 2017]: Local strong convexity of two layers NN.
- [Soudry, Carmon, 2016], [Ge, Lee, Ma, 2017], [Tian, 2017], [Soltanolkotabi, 2017], [Li, Yuan, 2017] ...
Mean field perspective: Emp. dist. of weights

- Prediction function
  \[
  f(x; \theta) = \frac{1}{N} \sum_{i=1}^{N} \sigma_{\bullet}(x; \theta_i) = \int \sigma_{\bullet}(x; \theta) \hat{\rho}_N(d\theta).
  \]

- Empirical distribution of the weights:
  \[
  \hat{\rho}_N = \frac{1}{N} \sum_{i=1}^{N} \delta_{\theta_i} \in \mathcal{P}(\mathbb{R}^D).
  \]

- Risk functional \( R : \mathcal{P}(\mathbb{R}^D) \to \mathbb{R} \)
  \[
  R(\rho) = \mathbb{E}_{x,y} \left[ \ell(y, \int \sigma_{\bullet}(x; \theta) \rho(d\theta)) \right].
  \]
Induced dynamics on empirical distribution

- Gradient flow on particles $\{\theta^t_i\}_{i \in [N]}, \theta^t_i \in \mathbb{R}^D$,

$$\frac{d}{dt} \theta^t_i = -N \xi(t) \nabla_{\theta} R_N(\theta^t), \quad \theta^0_i = \theta^0_i.$$  \hspace{1cm} (GF)

- Define dynamics on distribution $\rho_{N,t} \in \mathcal{P}(\mathbb{R}^D)$,

$$\partial_t \rho_{N,t}(\theta) = 2\xi(t) \nabla_{\theta} \cdot (\rho_{N,t}(\theta) \nabla_{\theta} \Psi(\theta; \rho_{N,t})), \hspace{1cm} \text{(PDE)}$$

with

$$\rho_{N,0} = \frac{1}{N} \sum_{i=1}^{N} \delta_{\theta^0_i}, \quad \Psi(\theta; \rho) = \frac{\delta R}{\delta \rho}(\theta; \rho).$$

- Claim: $\rho_{N,t} = (1/N) \sum_{i=1}^{N} \delta_{\theta^t_i}$. 
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Particle Dynamics

\[ \frac{d}{dt} \theta_i^t = - \nabla_{\theta_i} R_N(\theta^t) \]

Distribution Dynamics

\[ a_t \rho_t = \nabla \cdot (\rho_t \nabla \Phi(\theta; \rho_t)) \]
A short proof

Test function + Chain rule + Integration by part.

\[
\frac{d}{dt} \int f(\theta) \rho_{N,t}(d\theta) = \frac{d}{dt} \left[ \frac{1}{N} \sum_{i=1}^{N} f(\theta_i^t) \right] = - \frac{1}{N} \sum_{i=1}^{N} \langle \nabla f(\theta_i^t), N \nabla_{\theta} R_N(\theta^t) \rangle
\]

\[= - \frac{1}{N} \sum_{i=1}^{N} \langle \nabla f(\theta_i^t), \nabla[\delta R/\delta \rho](\theta_i^t; \rho_{N,t}) \rangle \]

\[= - \int \langle \nabla f, \nabla[\delta R/\delta \rho](\theta; \rho_{N,t}) \rangle \rho_{N,t}(d\theta). \]
What is this PDE?

\[ \partial_t \rho_t = \nabla_\theta \cdot (\rho_t \nabla_\theta \Psi(\theta; \rho_t)). \]

Existence and uniqueness: [Sznitman, 1991].

- **Physics:** nonlinear transport equation describing motions of particles with pairwise interaction (mean field approach).

- **Math:** Gradient flow of \( R(\rho) \) in the metric space \( (\mathcal{P}(\mathbb{R}^D), W_2) \). [Jordan, Kinderlehrer, Otto, 1998], [Ambrosio, Gigli, Savaré, 2006], [Carrillo, McCann, Villani, 2013]
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Converge of $\rho_{N,t}$ to $\rho_t$ as $N \to \infty$

Let $\rho_{N,t}$ be the solution of $(\theta^0_i \sim iid \ rho_0 \in \mathcal{P}(\mathbb{R}^D))$

$$\partial_t \rho_{N,t} = \nabla_{\theta} \cdot \left( \rho_{N,t} \nabla_{\theta} \Psi(\theta; \rho_{N,t}) \right), \quad \rho_{N,0} = \frac{1}{N} \sum_{i=1}^{N} \delta_{\theta^0_i}.$$

Let $\rho_t$ be the solution of

$$\partial_t \rho_t = \nabla_{\theta} \cdot \left( \rho_t \nabla_{\theta} \Psi(\theta; \rho_t) \right), \quad \rho_t |_{t=0} = \rho_0.$$
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Converge of $\rho_{N,t}$ to $\rho_t$ as $N \to \infty$

Theorem (M., Montanari, and Nguyen, 2018)

Under some assumptions. Let $(\theta^0_i)_{i \leq N} \sim_{iid} \rho_0$. Denote $\rho_{N,t}$: emp. dist. of sol. of grad. flow with init. $\theta^0$. Denote $\rho_t$: sol. of PDE with init. $\rho_0$. Then, $\forall f$ bounded Lipschitz,

$$\sup_{t \leq T} \left| \int f(\theta) \rho_{N,t}(d\theta) - \int f(\theta) \rho_t(d\theta) \right| \leq Ke^{KT} \sqrt{\frac{\log(N/\delta)}{N}}$$

with probability at least $1 - \delta$.

- See also [Rotskoff, Vanden-Eijnden, 2018], [Sirignano, Spiliopoulos, 2018].
Immediate implication

\[ \rho_{N,t} \to \rho_t, \quad N \to \infty \]

\[ \partial \rho_t = \nabla \cdot \left( \rho_t \nabla \Psi(\theta; \rho_t) \right), \quad \rho_t|_{t=0} = \rho_0. \]

Convergence speed of \( N \)-neuron gradient flow is independent of \( N \! \! \! \! . \)

- Effective dimension from \( N \times D \) to \( D \).
SGD v.s. PDE

![Graphs showing the comparison between SGD and PDE at different iterations](image)

- **Iteration 10^3**
- **Iteration 4 \times 10^6**
- **Iteration 10^7**
Does $R(\rho_t) \rightarrow \min_\rho R(\rho)$ as $t \rightarrow \infty$?

In general, no convergence guarantees.

But sometimes, yes.

[M., Montanari, Nguyen, 2018]

- Case by case: a special mixture of two Gaussians.
- Noisy SGD (PDE with diffusion term).
PDE with diffusion term

Noisy gradient flow

$$d\theta^t_i = -N\nabla_{\theta_i} R_N(\theta^t_i)dt + \frac{1}{\sqrt{\beta}}dW^t_i.$$ 

PDE with diffusion term

$$\partial_t \rho_t = \nabla_{\theta} \cdot \left( \rho_t \nabla_{\theta} \Psi(\theta; \rho_t) \right) + \frac{1}{\beta} \Delta \rho_t. \quad (\star)$$

Wasserstein grad. flow of the free energy

$$F_\beta(\rho) = R(\rho) + \frac{1}{\beta} \int \rho(\theta) \log \rho(\theta) d\theta.$$

**Theorem (M., Montanari, Nguyen, 2018)**

\((\star)\) converges to the minimizer of \(F_\beta(\rho)\) as \(t \to \infty\).
General convergence for noisy SGD

Theorem (M., Montanari, Nguyen, 2018)

Under certain assumptions. Initialization $(\theta^0_i)_{i \leq N} \sim \text{iid } \rho_0$. Then there exists $\beta_0 = \beta_0(D,U,V,\eta)$, such that, for $\beta \geq \beta_0$, there exists $T = T(D,U,V,\beta,\eta)$ such that for any $k \in [T/\varepsilon, 10T/\varepsilon]$, $N \geq C_0 D \log D$, $\varepsilon \leq 1/(C_0 D)$, we have, w.h.p.

$$R_{\lambda,N}(\theta^k) \leq \inf_{\theta \in \mathbb{R}^{D \times N}} R_{\lambda,N}(\theta) + \eta.$$

- Cautious: no polynomial convergence rate.
General convergence for noisy SGD

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- Cautious: no polynomial convergence rate.
Still many open problems: establish global convergence, extend to multi-layers.
Agenda

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3. Transitions between mean field and tangent kernel regime
The neural tangent model

- Multi-layers neural network $f(x; \theta)$

\[
f(x; \theta) = \sigma(W_L\sigma(\cdots W_2\sigma(W_1x))).
\]

- Linearization around random parameter $\theta_0$

\[
f(x; \theta) = f(x; \theta_0) + \langle \theta - \theta_0, \nabla_\theta f(x; \theta_0) \rangle + o(\|\theta - \theta_0\|_2).
\]

- NT model: the linear part of $f$

\[
f_{NT}(x; \theta) = \langle \theta - \theta_0, \nabla_\theta f(x; \theta_0) \rangle.
\]
The neural tangent model

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- **NT model**: the linear part of $f$
  
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- **Random feature map**: $\nabla_\theta f(x; \theta_0)$.

- **Neural tangent kernel**: $\mathcal{K}_{NT}(x, y) = \langle \nabla_\theta f(x; \theta_0), \nabla_\theta f(y; \theta_0) \rangle$. [Jacot, Gabriel, Hongler, 2018], [Du, Zhai, Poczos, Singh, 2018], [Chizat, Bach, 2018b], ....

- **Successful optimization**: under certain conditions (different from the mean field theory), the trajectory (of GF on empirical risk) of NT and NN is uniformly close.

Does NT models fully explain the success of neural networks?
The neural tangent model

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- **Successful optimization**: under certain conditions (different from the mean field theory), the trajectory (of GF on empirical risk) of NT and NN is uniformly close.

Does NT models fully explain the success of neural networks?
Empirically, the generalization of NT models are not as good as NN

**Table:** Cifar10 experiments

<table>
<thead>
<tr>
<th>Architecture</th>
<th>Classification error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Best convolutional NN</td>
<td>5%</td>
</tr>
<tr>
<td>Best convolutional NT</td>
<td>23%</td>
</tr>
<tr>
<td>CNN of best CNT</td>
<td>19%</td>
</tr>
</tbody>
</table>

[Arora, Du, Hu, Li, Salakhutdinov, Wang, 2019]
Theoretical analysis of generalization gap

Two-layers neural network

\[ f_N(x; \Theta) = \sum_{i=1}^{N} a_i \sigma(\langle w_i, x \rangle), \quad \Theta = (a_1, w_1, \ldots, a_N, w_N). \]

- Input vector \( x \in \mathbb{R}^d \).
- Bottom layer weights \( w_i \in \mathbb{R}^d, i = 1, 2, \ldots, N \).
- Top layer weights \( a_i \in \mathbb{R}, i = 1, 2, \ldots, N \).
Random features model and Neural tangent model

Linearization

\[
f_N(x; \Theta) = f_N(x; \Theta^0) + \sum_{i=1}^{N} \Delta a_i \sigma(\langle w_i^0, x \rangle) + \sum_{i=1}^{N} a_i^0 \sigma'(\langle w_i^0, x \rangle) \langle \Delta w_i, x \rangle + o(\cdot).
\]

Second layer linearization

First layer linearization

Linearized neural network: \((w_i \sim \text{Unif}(S^{d-1}))\)

\[
\mathcal{F}_{RF,N}(W) = \left\{ f = \sum_{i=1}^{N} a_i \sigma(\langle w_i, x \rangle) : a_i \in \mathbb{R}, i \in [N] \right\},
\]

\[
\mathcal{F}_{NT,N}(W) = \left\{ f = \sum_{i=1}^{N} \sigma'(\langle w_i, x \rangle) \langle a_i, x \rangle : a_i \in \mathbb{R}^d, i \in [N] \right\}.
\]

Blue: random and fixed. Red: parameters to be optimized.
Approximation error

Data distribution:

\[ x \sim \text{Unif}(\mathbb{S}^{d-1}(\sqrt{d})), \quad f_\star \in L^2(\mathbb{S}^{d-1}(\sqrt{d})). \]

Minimum risk (approximation error):

\[
R_{M,N}(f_\star) = \inf_{f \in \mathcal{F}_{M,N}(W)} \mathbb{E}_x \left[ (f_\star(x) - f(x))^2 \right], \quad M \in \{\text{RF, NT}\}.
\]
Staircase lower bound
Lower bound for random features regression

\[ \mathcal{F}_{RF, N}(W) = \left\{ f = \sum_{i=1}^{N} a_i \sigma(\langle w_i, x \rangle) : a_i \in \mathbb{R}, i \in [N] \right\}. \]

**Theorem (Ghorbani, M., Misiakiewics, Montanari, 2019)**

Assume \( N = O_d(d^{\ell+1-\delta}) \), and \((w_i)_{i \in [N]} \sim \text{Unif}(S^{d-1})\), we have

\[
\inf_{f \in \mathcal{F}_{RF, N}(W)} \mathbb{E}_x [(f_*(x) - f(x))^2] \geq \|P_{>\ell} f_*\|_{L^2}^2 + o_d, \mathbb{P}(\|f_*\|_2^2).
\]

\( P_{>\ell} \): projection orthogonal to the space of degree-\( \ell \) polynomials.

With \( N = O_d(d^{k}) \) parameters, one can only fit a degree \( k \) polynomial.
Lower bound for random features regression

\[ \mathcal{F}_{RF, N}(W) = \left\{ f = \sum_{i=1}^{N} a_i \sigma(\langle w_i, x \rangle) : a_i \in \mathbb{R}, i \in [N] \right\}. \]

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\[ \inf_{f \in \mathcal{F}_{RF, N}(W)} \mathbb{E}_x [(f_\ast(x) - f(x))^2] \geq \|P_{>\ell} f_\ast\|_{L^2}^2 + o_d, \mathbb{P}(\|f_\ast\|_2^2). \]

\( P_{>\ell} \): projection orthogonal to the space of degree-\( \ell \) polynomials.

With \( N = O_d(d^k) \) parameters, one can only fit a degree \( k \) polynomial.
Similar result for NT

\[ \mathcal{F}_{NT, N}(W) = \left\{ f = \sum_{i=1}^{N} \sigma'(\langle w_i, x \rangle) \langle a_i, x \rangle : a_i \in \mathbb{R}^d, i \in [N] \right\}. \]

**Theorem (Ghorbani, M., Misiakiewics, Montanari, 2019)**

Assume \( N = O_d(d^{\ell+1-\delta}) \), and \((w_i)_{i \in [N]} \sim \text{Unif}(S^{d-1})\), we have

\[
\inf_{f \in \mathcal{F}_{NT, N}(W)} \mathbb{E}_x [(f_\star(x) - f(x))^2] \geq \|P_{>\ell+1} f_\star\|_{L^2}^2 + o_d, \mathbb{P}(\|f_\star\|_2^2),
\]

\( P_{>\ell+1} \): projection orthogonal to the space of degree-\((\ell + 1)\) polynomials.

With \( O_d(d^{k+1}) \) parameters, one can only fit a degree \( k + 1 \) polynomial.
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\]

\( P_{\ell+1} : \) projection orthogonal to the space of degree-(\( \ell + 1 \)) polynomials.

With \( O_d(d^{k+1}) \) parameters, one can only fit a degree \( k + 1 \) polynomial.
The staircase lower bound

\[ f = P_0 f + P_1 f + P_2 f + P_3 f + \cdots \]
Implication

Function $f : \mathbb{S}^{d-1} \to \mathbb{R}, f(x) = P_k(x_1)$.

- **NT**: $N \geq \Theta_d(d^{k-1})$;
- **NN**: $N = O_d(1)$.

Different from the RKHS theory [Bach, 2017], [E, Ma, Wu, 2018].

- **Difference 1**: $f_\star \in L^2$, v.s. $f_\star \in$ RKHS.

- **Difference 2**: $N = d^k$ as $d \to \infty$, v.s. fixed $d$ as $N \to \infty$. 
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- Difference 1:
  \[ f_* \in L^2, \quad \text{v.s.} \quad f_* \in \text{RKHS}. \]
- Difference 2:
  \[ N = d^k \text{ as } d \to \infty, \quad \text{v.s.} \quad \text{fixed } d \text{ as } N \to \infty. \]
double descent curve
Experiment setup

- **MNIST dataset**: $(x, y) \in \mathbb{R}^{100} \times [10]$. Training/test data size: 50000/10000.

- **Two-layers neural networks**:

  \[
  f_N(x; \Theta) = \sum_{i=1}^{N} a_i \sigma(\langle w_i, x \rangle), \quad \Theta = (a_1, w_1, \ldots, a_N, w_N).
  \]

  Bottom layer weights $w_i \in \mathbb{R}^{100}$. Top layer weights $a_i \in \mathbb{R}$.

- **Loss function**: cross entropy. Training algorithm: SGD.

- $N$: model complexity, to be varied.
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Experimental results

Figure: Experiments on MNIST. Left: [Spigler, Geiger, Ascoli, Sagun, Biroli, Wyart, 2018]. Right: [Belkin, Hsu, Ma, Mandal, 2018]. See also: [Neyshabur, Tomioka, Srebro, 2014a].
Double descent

![Diagram of double descent](image)

- Peak at the interpolation threshold.
- Monotonic decreasing in the overparameterized regime.
- Global minimum when the number of parameters is infinity.

**Figure:** A cartoon by [Belkin, Hsu, Ma, Mandal, 2018].
Linear model with random covariates

By [Hastie, Montanari, Rosset, Tibshirani, 2019]. See also [Belkin, Hsu, Xu, 2019].

Model: \( y = \langle x, \beta^* \rangle + \epsilon, \ x \sim \mathcal{N}(0, I_d) \).

Loss: \( L(\beta) = \hat{E}[(y - \langle x, \beta \rangle)^2] \)
Why singularity?

- Model: $x_i \sim \mathcal{N}(0, I_d)$, $y_i = \langle x_i, \beta_\star \rangle + \varepsilon_i$, $\beta_\star = 0$, $i \in [n]$.

- Test risk $\propto \mathbb{E}[\|\hat{\beta}\|^2_2] \propto \mathbb{E}[\|X^\top y\|^2_2] \propto \mathbb{E}[\text{tr}((X^\top X)^\top)]$.

- When $n \neq d$, $X$ is well conditioned.

- When $n \approx d$, $X$ is infinitely ill conditioned.

- The model has marginally enough parameters to interpolate all the data, hence it interpolates in an awkward way.

- To fit the noise, the coefficients $\|\hat{\beta}\|^2_2 = \|X^\top y\|^2_2$ blows up.
Why singularity?

- Model: $x_i \sim \mathcal{N}(0, I_d)$, $y_i = \langle x_i, \beta_* \rangle + \varepsilon_i$, $\beta_* = 0$, $i \in [n]$.

- Test risk $\propto \mathbb{E}[\|\hat{\beta}\|_2^2] \propto \mathbb{E}[\|X^\top y\|_2^2] \propto \mathbb{E}[\text{tr}((X^\top X)^\dagger)]$.

- When $n \neq d$, $X$ is well conditioned.

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- To fit the noise, the coefficients $\|\hat{\beta}\|_2^2 = \|X^\top y\|_2^2$ blows up.
✓ Peak at the interpolation threshold.
?
Monotonic decreasing in the overparameterized regime.
?
Global minimum when the number of parameters is infinity.
Goal: find a tractable model that exhibits all the features of the double descent curve.

Figure: By [Belkin, Hsu, Ma, Mandal, 2018].
A simple model

The random features model

\[ f_{RF}(x; a) = \sum_{j=1}^{N} a_j \sigma(\langle w_j, x \rangle). \]

Random weights

\[ w_j \sim_{iid} \text{Unif}(S^{d-1}). \]
Random features regression: \( \hat{a}_\lambda = \arg \min_a L_\lambda(a) \),

\[
L_\lambda(a) = \frac{1}{n} \sum_{i=1}^{n} \left[ \left( y_i - \sum_{j=1}^{N} a_j \sigma(\langle x_i, w_j \rangle) \right)^2 \right] + \frac{\lambda N}{d} \| a \|_2^2,
\]

\[
R(a; f_\star) = \mathbb{E}_{x,y} \left[ \left( f_\star(x) - \sum_{j=1}^{N} a_j \sigma(\langle x, w_j \rangle) \right)^2 \right].
\]

Data: \((x_i)_{i \in [n]} \sim \text{Unif}(S^{d-1}(\sqrt{d}))\), \(y_i = f_\star(x_i) + \varepsilon_i\), \(\mathbb{E}[\varepsilon_i^2] = \tau^2\).

Weights: \((w_j)_{j \in [N]} \sim_{iid} \text{Unif}(S^{d-1})\).

Activation \(\sigma\): \(\| P_1 \sigma \|_{L^2}^2 = \mu_1^2\), and \(\| P_{>1} \sigma \|_{L^2}^2 = \mu_\star^2\).

Tech. ass. on \(f_\star\) and \(\sigma\). Almost every nonlinear \(f_\star\) and \(\sigma\).

\(n\) data, \(N\) features, \(d\) dimension. \(N/d \to \psi_1\), \(n/d \to \psi_2\), as \(d \to \infty\).
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\]

\[
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Weights: \( (w_j)_{j\in[N]} \sim \text{iid Unif}(S^{d-1}). \)

Activation \( \sigma: \|P_1 \sigma\|_{L^2}^2 = \mu_1^2, \) and \( \|P_{>1} \sigma\|_{L^2}^2 = \mu_\sigma^2. \)

Tech. ass. on \( f^* \) and \( \sigma. \) Almost every nonlinear \( f^* \) and \( \sigma. \)

\( n \) data, \( N \) features, \( d \) dimension. \( N/d \rightarrow \psi_1, n/d \rightarrow \psi_2, \) as \( d \rightarrow \infty. \)
Setting

- Random features regression: \( \hat{a}_\lambda = \arg\min_{a} L_\lambda(a) \),

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\]

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\[
R(a; f_*) = \mathbb{E}_{x,y} \left[ (f_*(x) - \sum_{j=1}^{N} a_j \sigma(\langle x, w_j \rangle))^2 \right].
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Activation $\sigma$: $\|P_1 \sigma\|_{L^2}^2 = \mu_1^2$, and $\|P_{>1} \sigma\|_{L^2}^2 = \mu_\star^2$.

Technical ass. on $f_\star$ and $\sigma$. Almost every nonlinear $f_\star$ and $\sigma$.

$n$ data, $N$ features, $d$ dimension. $N/d \to \psi_1$, $n/d \to \psi_2$, as $d \to \infty$. 
Precise asymptotics

Random features regression: \( \hat{a}_\lambda = \arg \min_a L_\lambda(a) \),

\[
R(a; f_*) = E_{x,y} \left[ \left( f_*(x) - \sum_{j=1}^N a_j \sigma(\langle x, w_j \rangle) \right)^2 \right].
\]

**Theorem (M. and Montanari, 2019)**

Under above assumptions, for any \( \lambda > 0 \), we have

\[
R(\hat{a}_\lambda; f_*) = \|P_{\text{lin}} f_*\|_{L^2}^2 \cdot B(\zeta, \psi_1, \psi_2, \lambda/\mu_*^2) + (\tau^2 + \|P_{\text{nl}} f_*\|_{L^2}^2) \cdot V(\zeta, \psi_1, \psi_2, \lambda/\mu_*^2) + o_d, P(1),
\]

where functions \( B \) and \( V \) are given explicitly below.

(Similar result for the training error. )
Explicit formulae

Let the functions $\nu_1, \nu_2 : \mathbb{C}_+ \rightarrow \mathbb{C}_+$ be the unique solution of

$$
\nu_1 = \psi_1 \left( -\xi - \nu_2 - \frac{\zeta^2 \nu_2}{1 - \zeta^2 \nu_1 \nu_2} \right)^{-1},
$$

$$
\nu_2 = \psi_2 \left( -\xi - \nu_1 - \frac{\zeta^2 \nu_1}{1 - \zeta^2 \nu_1 \nu_2} \right)^{-1};
$$

Let

$$
\chi \equiv \nu_1 (i(\psi_1 \psi_2 \bar{\lambda})^{1/2}) \cdot \nu_2 (i(\psi_1 \psi_2 \bar{\lambda})^{1/2}),
$$

and

$$
\mathcal{E}_0(\zeta, \psi_1, \psi_2, \bar{\lambda}) \equiv -\chi^5 \zeta^6 + 3\chi^4 \zeta^4 + (\psi_1 \psi_2 - \psi_2 - \psi_1 + 1)\chi^3 \zeta^6 - 2\chi^3 \zeta^4 - 3\chi^3 \zeta^2
$$

$$
+ (\psi_1 + \psi_2 - 3\psi_1 \psi_2 + 1)\chi^2 \zeta^4 + 2\chi^2 \zeta^2 + \chi^2 + 3\psi_1 \psi_2 \chi^2 - \psi_1 \psi_2,
$$

$$
\mathcal{E}_1(\zeta, \psi_1, \psi_2, \bar{\lambda}) \equiv \psi_2 \chi^3 \zeta^4 - \psi_2 \chi^2 \zeta^2 + \psi_1 \psi_2 \chi \zeta^2 - \psi_1 \psi_2,
$$

$$
\mathcal{E}_2(\zeta, \psi_1, \psi_2, \bar{\lambda}) \equiv \chi^5 \zeta^6 - 3\chi^4 \zeta^4 + (\psi_1 - 1)\chi^3 \zeta^6 + 2\chi^3 \zeta^4 + 3\chi^3 \zeta^2 + (-\psi_1 - 1)\chi^2 \zeta^4 - 2\chi^2 \zeta^2 - \chi^2.
$$

We then have

$$
\mathcal{B}(\zeta, \psi_1, \psi_2, \bar{\lambda}) \equiv \frac{\mathcal{E}_1(\zeta, \psi_1, \psi_2, \bar{\lambda})}{\mathcal{E}_0(\zeta, \psi_1, \psi_2, \bar{\lambda})},
$$

$$
\mathcal{V}(\zeta, \psi_1, \psi_2, \bar{\lambda}) \equiv \frac{\mathcal{E}_2(\zeta, \psi_1, \psi_2, \bar{\lambda})}{\mathcal{E}_0(\zeta, \psi_1, \psi_2, \bar{\lambda})}.
$$
Insights
✓ Peak at the interpolation threshold.
✓ Monotonic decreasing in the overparameterized regime.
✓ Global minimum when the number of parameters is infinity.
- For any $\lambda$, the min prediction error is achieved at $N/n \to \infty$.
- For optimal $\lambda$, the prediction error is monotonically decreasing.
- High SNR: minimum at $\lambda = 0+$;
- Low SNR: minimum at $\lambda > 0$. 
Agenda

1. Mean field theory

2. Tangent kernel theory

3. Transitions between mean field and tangent kernel regime
Connections of mean field and tangent kernel

Setup: $\alpha$ controls the speed of change of emp. dist.

Prediction function: \[
\hat{f}_{\alpha,N}(x; \theta) = \frac{\alpha}{N} \sum_{j=1}^{N} \sigma_j(x; \theta_j),
\]

Risk function: \[
R_{\alpha,N}(\theta) = \mathbb{E}_x \left[ \left( f(x) - \hat{f}_{\alpha,N}(x; \theta) \right)^2 \right],
\]

Gradient flow: \[
\frac{d\theta_j^t}{dt} = - \frac{N}{2\alpha^2} \nabla_{\theta_j} R_{\alpha,N}(\theta^t).
\]
The coupled dynamics

Denote $\rho_t^{\alpha,N} = (1/N) \sum_{j=1}^{N} \delta_{\theta_j^t}$. Distributional dynamics:

$$\partial_t \rho_t^{\alpha,N} = (1/\alpha) \nabla_{\theta} \cdot (\rho_t^{\alpha,N} \nabla_{\theta} \Psi(\theta; \rho_t^{\alpha,N})).$$

Denote $u_t^{\alpha,N}(z) = f(z) - \hat{f}_{\alpha,N}(z; \theta^t)$. Residual dynamics:

$$\partial_t \|u_t^{\alpha,N}\|_{L^2}^2 = - \langle u_t^{\alpha,N}, \mathcal{H}_{\rho_t^{\alpha,N}} u_t^{\alpha,N} \rangle.$$

Here

$$\mathcal{H}_\rho(x,z) \equiv \int \langle \nabla_{\theta} \sigma_\ast(x; \theta), \nabla_{\theta} \sigma_\ast(z; \theta) \rangle \rho(d\theta),$$

$$\Psi_\alpha(\theta; \rho^{\alpha,N}) = - \mathbb{E}_x [u_t^{\alpha,N}(x) \sigma_\ast(x; \theta)].$$

[Rotskoff, Vanden-Eijnden, 2018], [Chizat, Bach, 2018b]
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The coupled dynamics

Denote $\rho_{t}^{\alpha,N} = (1/N) \sum_{j=1}^{N} \delta_{\theta_{j}}$. Distributional dynamics:

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Here

$$\mathcal{H}_{\rho}(x, z) \equiv \int \langle \nabla_{\theta} \sigma_{\star}(x; \theta), \nabla_{\theta} \sigma_{\star}(z; \theta) \rangle \rho(d\theta),$$

$$\Psi_{\alpha}(\theta; \rho^{\alpha,N}) = -\mathbb{E}_{x}[u_{t}^{\alpha,N}(x) \sigma_{\star}(x; \theta)].$$

[Rotskoff, Vanden-Eijnden, 2018], [Chizat, Bach, 2018b]
The mean field limit and tangent kernel limit

\[ \partial_t \rho_t^{\alpha,N} = \left( \frac{1}{\alpha} \right) \nabla_{\theta} \cdot \left( \rho_t^{\alpha,N} \left[ \nabla_{\theta} \Psi(\theta; \rho_t^{\alpha,N}) \right] \right), \]
\[ \partial_t \| u_t^{\alpha,N} \|^2_{L^2} = - \langle u_t^{\alpha,N}, \mathcal{H}_{\rho_t^{\alpha,N}} u_t^{\alpha,N} \rangle. \]

▶ The mean field limit: fix \( \alpha = O(1) \) and let \( N \to \infty \).

▶ The tangent kernel limit: let \( \alpha = \sqrt{N} \to \infty \).

▶ In tangent kernel limit: the kernel will not change. The res. dynamics becomes self contained. The emp. risk converges to 0.
The mean field limit and tangent kernel limit

\[ \partial_t \rho_t^{\alpha,N} = \frac{1}{\alpha} \nabla_{\theta} \cdot (\rho_t^{\alpha,N} [\nabla_{\theta} \Psi(\theta; \rho_t^{\alpha,N})]), \]

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The mean field limit and tangent kernel limit

\[ \partial_t \rho_t^{\alpha,N} = \frac{1}{\alpha} \nabla \theta \cdot \left( \rho_t^{\alpha,N} \left[ \nabla \theta \Psi(\theta; \rho_t^{\alpha,N}) \right] \right), \]

\[ \partial_t \| u_t^{\alpha,N} \|^2_{L^2} = - \langle u_t^{\alpha,N}, H_{\rho_t^{\alpha,N}} u_t^{\alpha,N} \rangle. \]

- The mean field limit: fix \( \alpha = O(1) \) and let \( N \to \infty \).

- The tangent kernel limit: let \( \alpha = \sqrt{N} \to \infty \).

- In tangent kernel limit: the kernel will not change. The res. dynamics becomes self contained. The emp. risk converges to 0.
Benefits and limitations of the mean field theory

\[ \partial_t \rho_t = \nabla_\theta \cdot \left( \rho_t \nabla_\theta \Psi(\theta; \rho_t) \right). \]

Benefits:

- It captures the non-linear behavior of neural networks that potentially give better generalization.
- People believe in practice we are in this regime.

Limitations:

- Hard to prove convergence of PDE.
- Hard to generalize to multi-layers.
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Thanks!