Understanding Gradient Descent for Over-parameterized Deep Neural Networks

Marco Mondelli

Institute of Science and Technology Austria (IST Austria)

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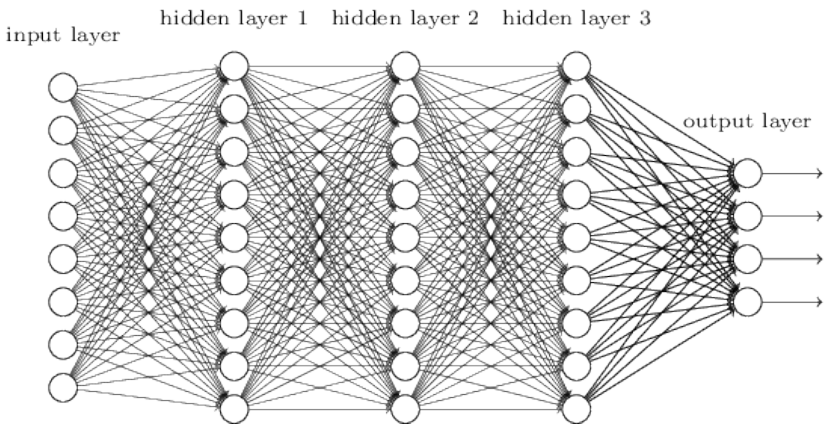
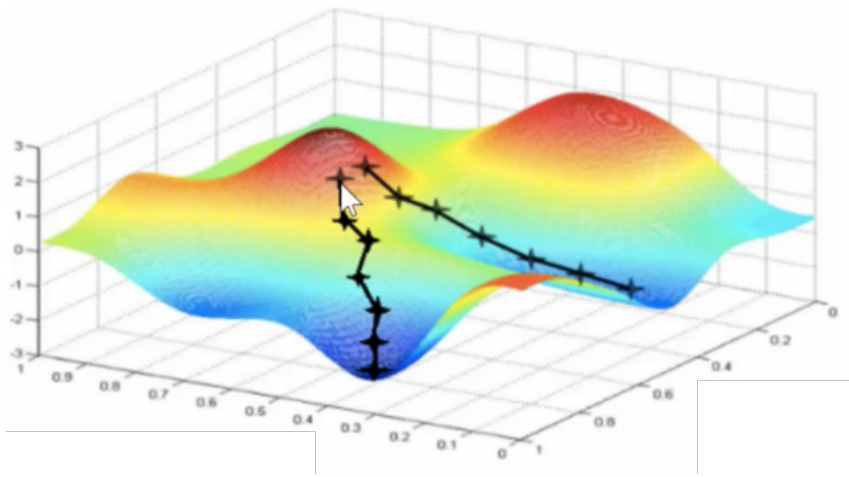
Training a neural network is difficult (NP-hardness, local/disconnected minima...), but it works remarkably well!

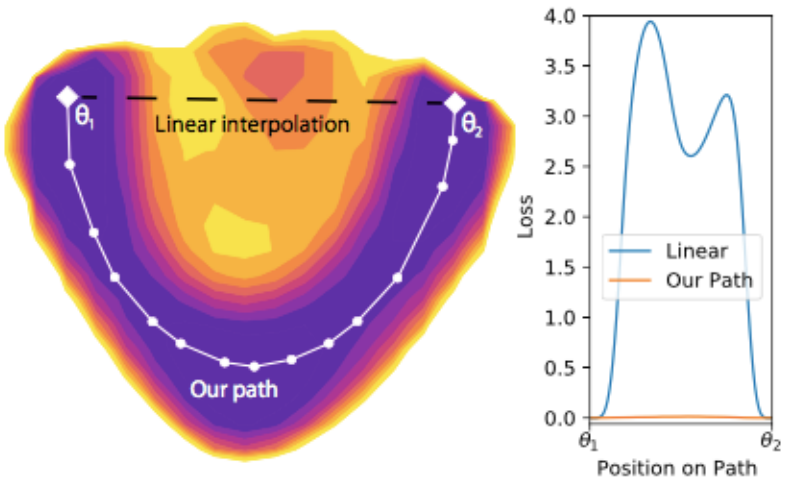




Over-parameterization

(Stochastic) gradient descent

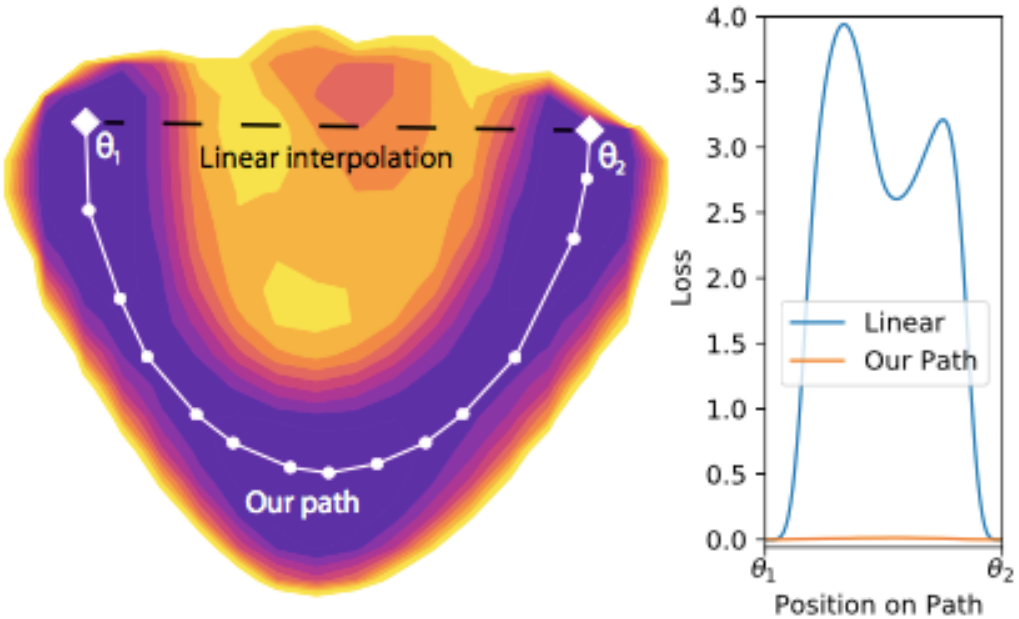
Landscape Connectivity and Dropout Stability



[SM20] A. Shevchenko and M. Mondelli, "Landscape Connectivity and Dropout Stability of SGD Solutions for Over-parameterized Neural Networks", *ICML*, 2020.

Landscape Connectivity

- SGD minima connected via piecewise linear path with constant loss [Garipov et al., 2018; Draxler et al., 2018]



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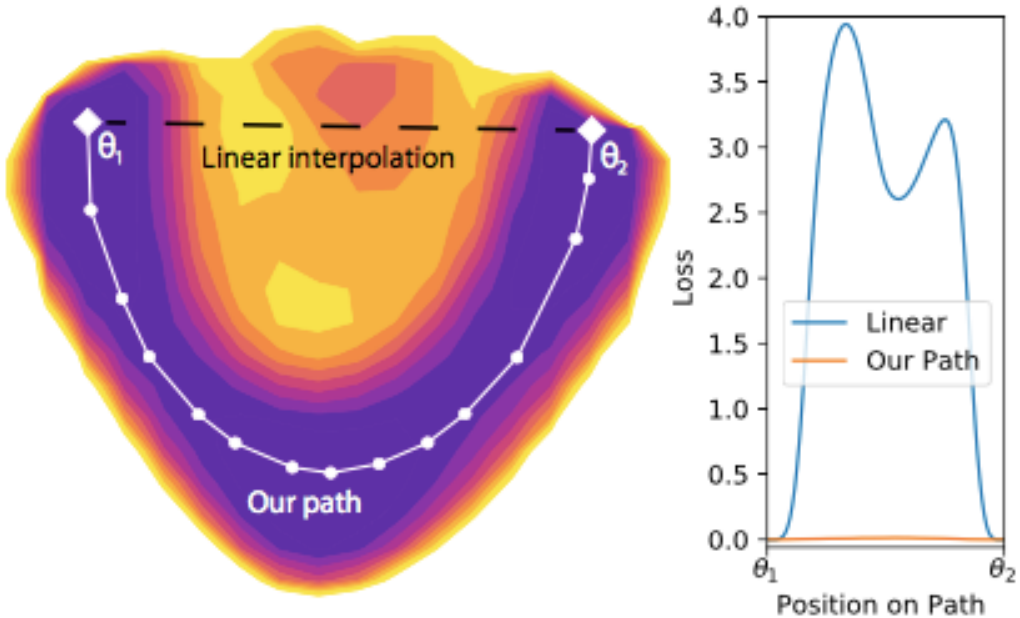
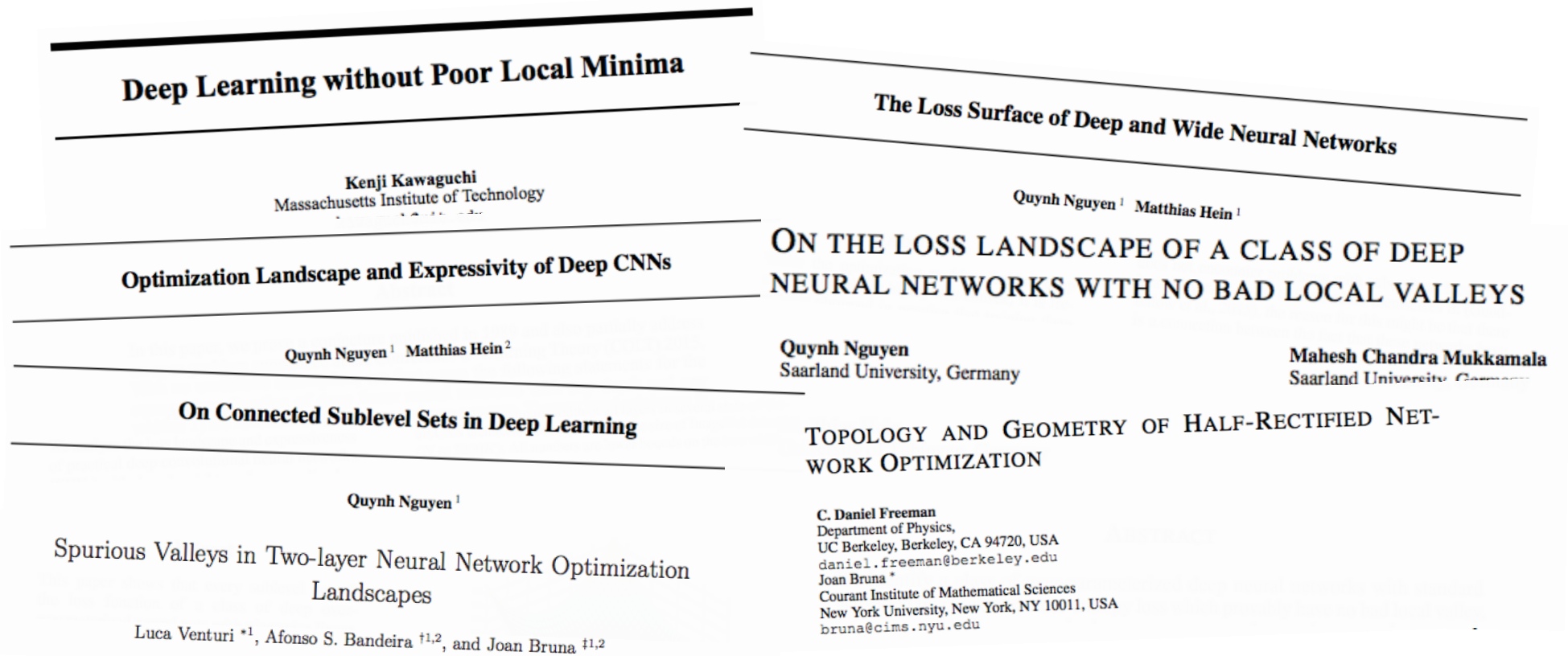


- Mode connectivity proved assuming properties of well-trained networks (dropout/noise stability) [Kuditipudi et al., 2019]

Landscape of Neural Networks

- Local minima are globally optimal for deep linear networks and networks with more neurons than training samples
- Connected sublevel sets for one wide layer and pyramidal topology
- Energy gap scaling exponentially with input dimension



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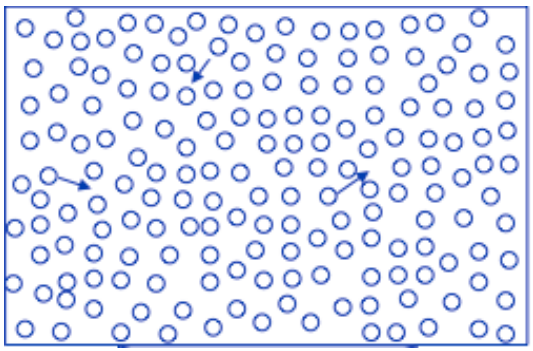
Strong assumptions on the model and **poor scaling** of parameters ☹

Mean Field View of Neural Networks



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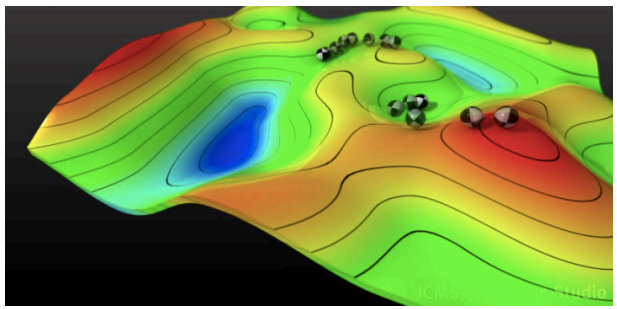

Discrete dynamics of SGD

Continuous dynamics of gradient flow

- Two layers [Mei et al., 2018; Rotskoff et al., 2018; Chizat et al., 2018; Sirignano et al., 2018; . . .]
- Multiple layers [Nguyen, 2019; Sirignano et al., 2019; Araujo et al., 2019]

Warm-Up: Two-Layer Networks

Data: $\{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_n, y_n)\} \sim_{\text{i.i.d.}} \mathbb{P}(\mathbb{R}^d \times \mathbb{R})$

Warm-Up: Two-Layer Networks

Data: $\{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_n, y_n)\} \sim_{\text{i.i.d.}} \mathbb{P}(\mathbb{R}^d \times \mathbb{R})$

Goal: Minimize loss $L_N(\boldsymbol{\theta}) = \mathbb{E}\left\{ \left(y - \frac{1}{N} \sum_{i=1}^{N} a_i \sigma(\boldsymbol{x}; \boldsymbol{w}_i) \right)^2 \right\}$, $\boldsymbol{\theta} = (\boldsymbol{w}, a)$

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Online SGD: $\boldsymbol{\theta}^{k+1} = \boldsymbol{\theta}^k + \alpha N \nabla_{\boldsymbol{\theta}^k} \left(\left(y_k - \frac{1}{N} \sum_{i=1}^{N} a_i^k \sigma(\boldsymbol{x}_k; \boldsymbol{w}_i^k) \right)^2 \right)$

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- y bounded, $\nabla_{\boldsymbol{w}} \sigma(\boldsymbol{x}; \boldsymbol{w})$ sub-gaussian
- σ bounded and differentiable, $\nabla\sigma$ bounded and Lipschitz
- initialization of a_i with bounded support

Dropout Stability

Dropout stability: loss does not change much if we remove part of neurons (and suitably rescale remaining neurons).

Dropout Stability

$$L_M(\boldsymbol{\theta}) = \mathbb{E}\left\{ \left(y - \frac{1}{M} \sum_{i=1}^{M} a_i \sigma(\boldsymbol{x}, \boldsymbol{w}_i) \right)^2 \right\}$$

$\boldsymbol{\theta}$ is ε_{D}-**dropout stable** if $|L_N(\boldsymbol{\theta}) - L_M(\boldsymbol{\theta})| \leq \varepsilon_{\mathrm{D}}$

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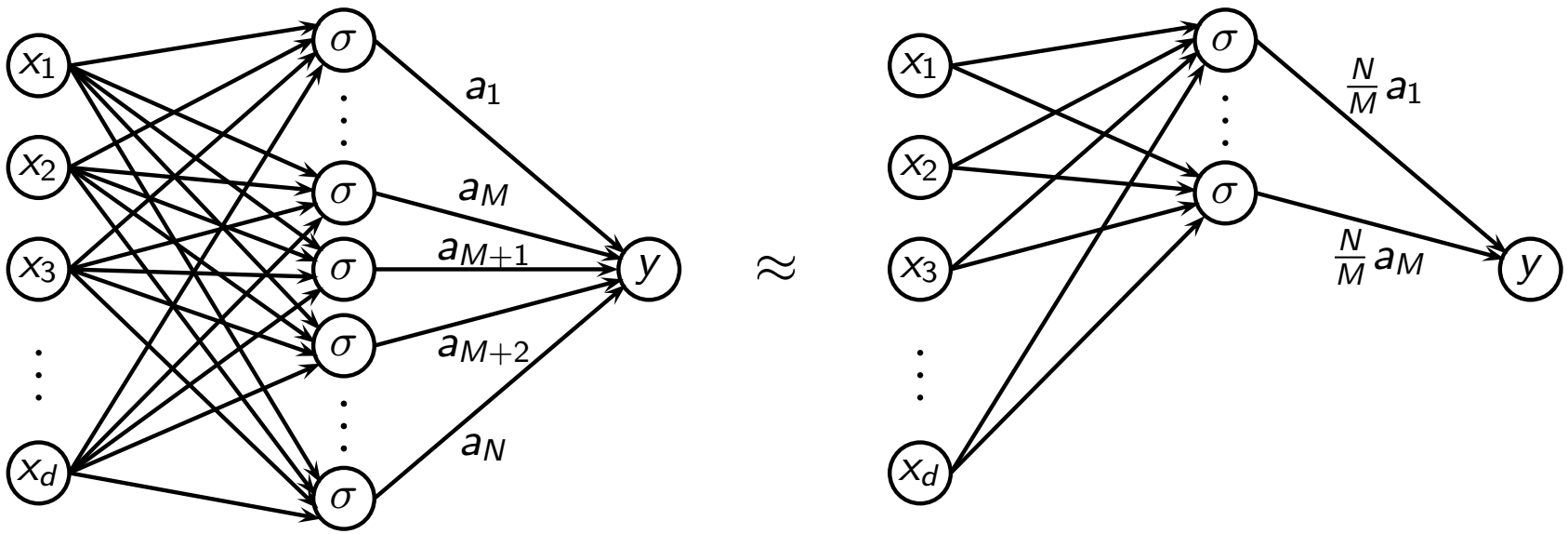

Dropout Stability and Connectivity

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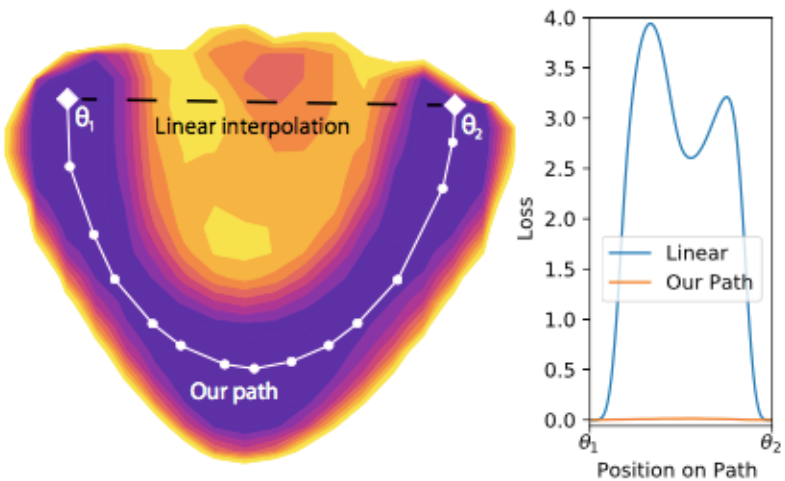

Dropout Stability, Provably

- $N = \#$ neurons of full network
- $M = \#$ neurons after dropout
- $\alpha =$ step size of SGD
- $D =$ dimension of weights

Theorem [SM20]

Let $\boldsymbol{\theta}^k$ be obtained after k SGD iterations. Then, with probability $1 - e^{-z^2}$, for all $k \in [T/\alpha]$, $\boldsymbol{\theta}^k$ is ε_{D}-dropout stable with

$$\varepsilon_{\mathrm{D}} = K e^{KT^3} \left(\frac{\sqrt{\log M} + z}{\sqrt{M}} + \sqrt{\alpha} \left(\sqrt{D + \log N} + z \right) \right).$$

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Change in loss scales as $\sqrt{\frac{\log M}{M}} + \sqrt{\alpha(D + \log N)}$

Connectivity, Provably

Theorem [SM20]

Let $\boldsymbol{\theta}^k$ be obtained after k SGD iterations using $\{(\boldsymbol{x}_j, y_j)\}_{j=0}^{k} \sim \mathbb{P}$, and $(\boldsymbol{\theta}')^{k'}$ after k' SGD iterations using $\{(\boldsymbol{x}'_j, y'_j)\}_{j=0}^{k'} \sim \mathbb{P}$.

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$$\varepsilon_{\mathrm{C}} = K e^{K \max(T,T')^3} \left(\frac{\sqrt{\log N} + z}{\sqrt{N}} + \sqrt{\alpha}\left(\sqrt{D + \log N} + z\right) \right).$$

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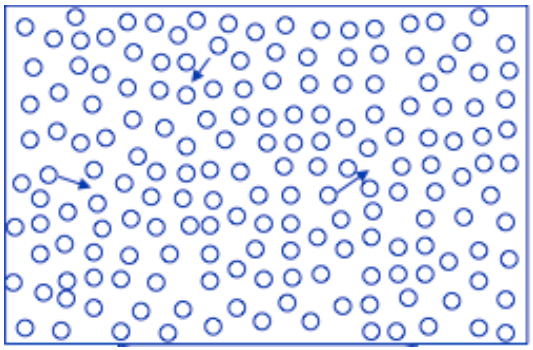
- Change in loss scales as $\sqrt{\frac{\log N}{N}} + \sqrt{\alpha(D + \log N)}$
- Can connect SGD solutions obtained from different training data (but same data distribution) and different initialization

Proof Idea



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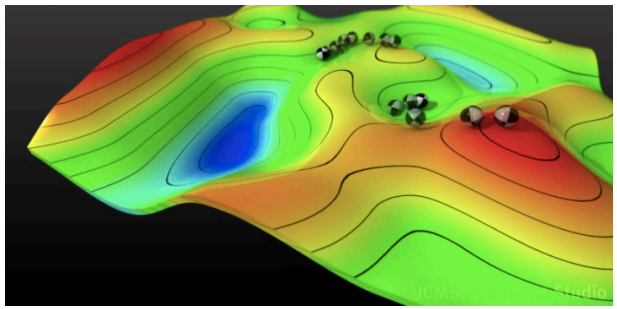

Discrete dynamics of SGD

Continuous dynamics of gradient flow

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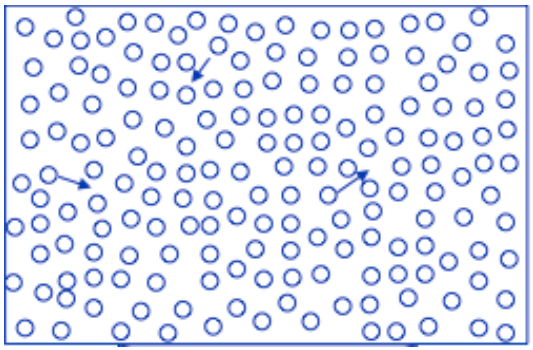

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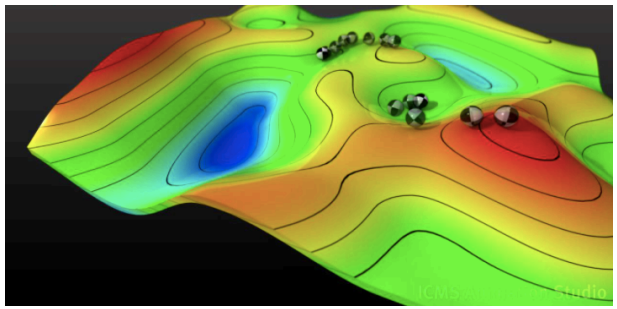

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- θ^k close to N i.i.d. particles that evolve with gradient flow

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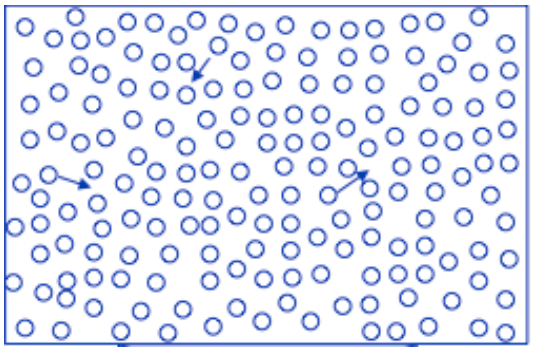

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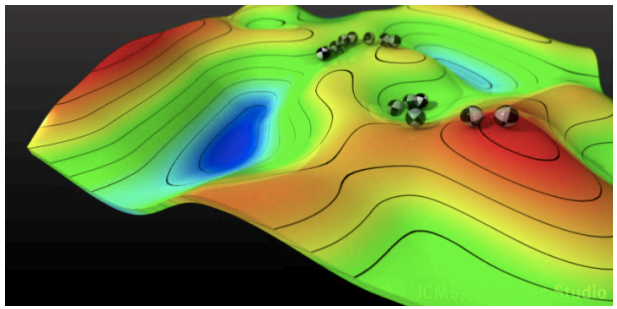

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- θ^k close to N i.i.d. particles that evolve with gradient flow
- $L_N(\theta^k)$ and $L_M(\theta^k)$ concentrate to the same limit

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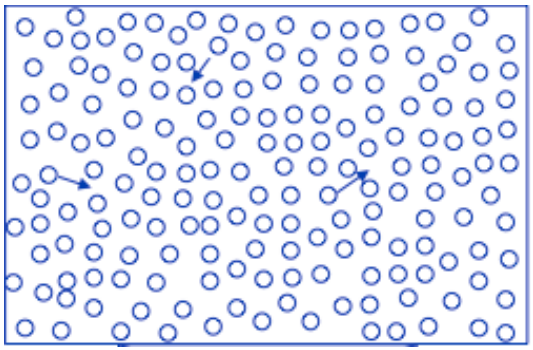

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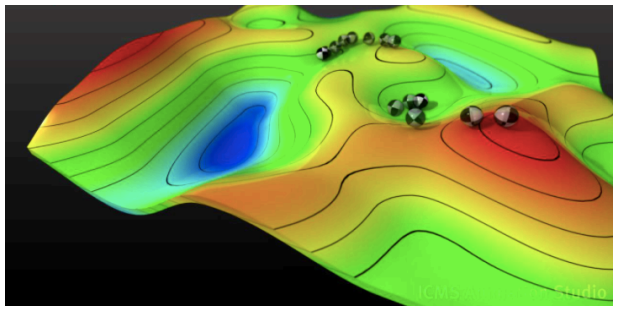


Discrete dynamics of SGD

Continuous dynamics of gradient flow

- $\boldsymbol{\theta}^k$ close to N i.i.d. particles that evolve with gradient flow
- $L_N(\boldsymbol{\theta}^k)$ and $L_M(\boldsymbol{\theta}^k)$ concentrate to the same limit
- Dropout stability with $M = N/2 \Rightarrow$ connectivity

Multilayer Networks

- $N = \#$ neurons per layer of full network
- $M =$ max. $\#$ neurons per layer after dropout
- $\alpha =$ step size of SGD
- $D = \max(d_x, d_y)$

Theorem [SM20]

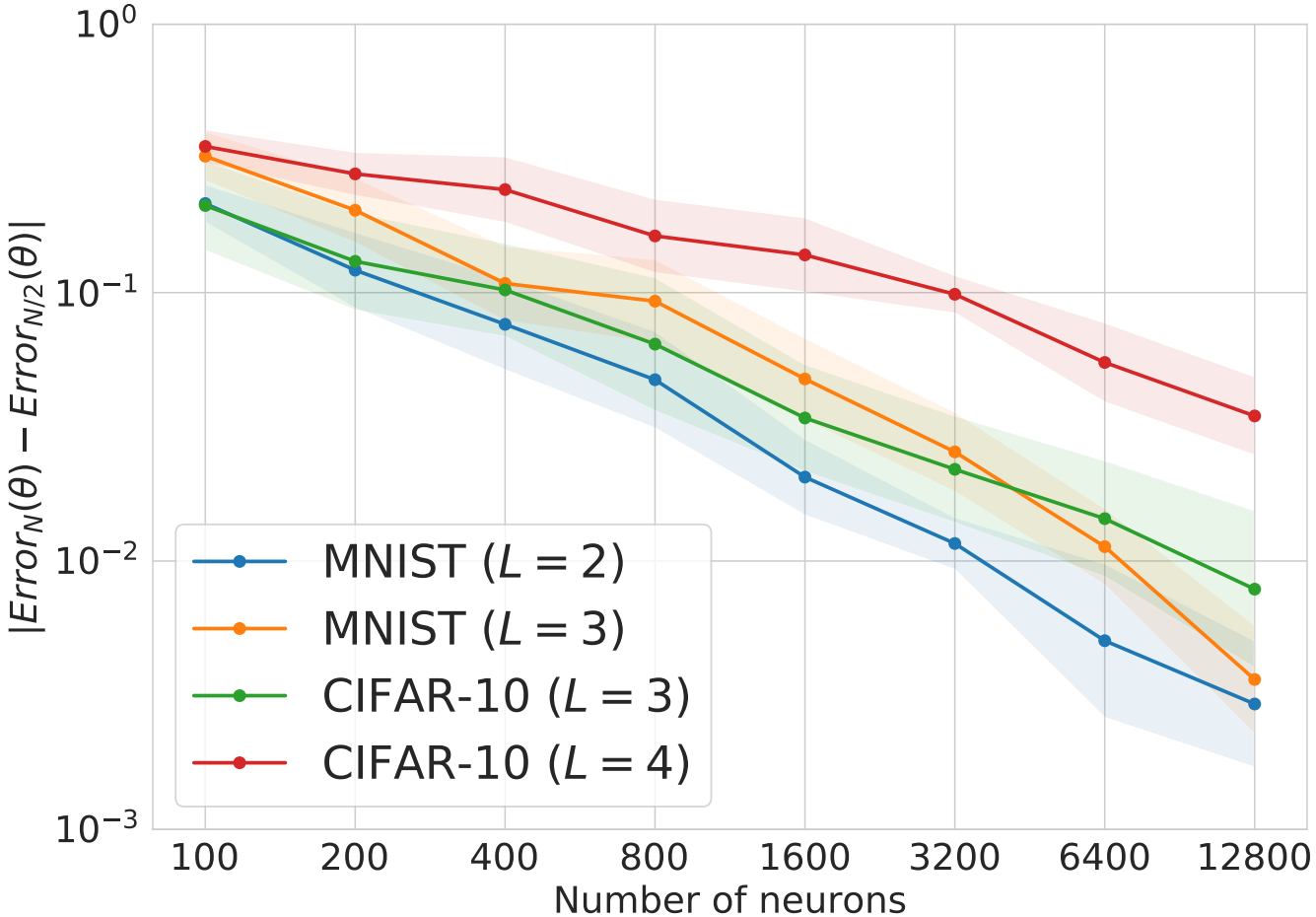
Let $\boldsymbol{\theta}^k$ be obtained after k SGD iterations, with $k = T/\alpha$. Then, w. p. $1 - e^{-z^2}$, $\boldsymbol{\theta}^k$ is ε_{D}-dropout stable with

$$\varepsilon_{\mathrm{D}} = K(T, L)\left(\frac{\sqrt{D} + z}{\sqrt{M}} + \frac{\sqrt{\log N}}{\sqrt{N}} + \sqrt{\alpha}\left(\sqrt{D + \log N} + z\right)\right).$$

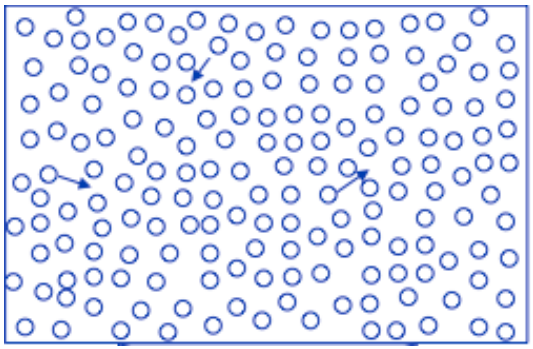
Let $(\boldsymbol{\theta}')^{k'}$ be obtained after k' SGD iterations, with $k' = T'/\alpha$. Then, w. p. $1 - e^{-z^2}$, $\boldsymbol{\theta}^k$ and $(\boldsymbol{\theta}')^{k'}$ are ε_{C}-connected with

$$\varepsilon_{\mathrm{C}} = K(T, T', L)\left(\frac{\sqrt{D + \log N} + z}{\sqrt{N}} + \sqrt{\alpha}\left(\sqrt{D + \log N} + z\right)\right).$$

Numerical Results



Global Convergence Without Rates



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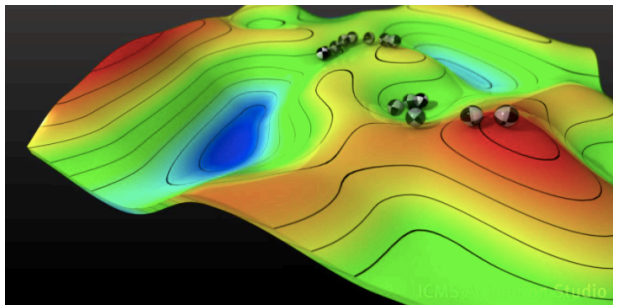

Discrete dynamics of SGD

Continuous dynamics of gradient flow

A mean field view of the landscape of two-layer neural networks

Song Mei[a], Andrea Montanari[b,c,1], and Phan-Minh Nguyen[b]

[a]Institute for Computational and Mathematical Engineering, Stanford University, Stanford, CA 94305; [b]Department of Electrical Engineering, Stanford University, Stanford, CA 94305; and [c]Department of Statistics, Stanford University, Stanford, CA 94305

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Multilayer neural networks are among the most powerful models in machine learning, yet the fundamental reasons for this success defy mathematical understanding. Learning a neural network requires optimizing a nonconvex high-dimensional objective (risk function), a problem that is usually attacked using stochastic gra-

present case, this amounts to the iteration

$$\theta_i^{k+1} = \theta_i^k + 2\varepsilon_k \left(y_k - \hat{y}(\boldsymbol{x}_k; \boldsymbol{\theta}^k)\right) \nabla_{\theta_i} \sigma_*(\boldsymbol{x}_k; \theta_i^k). \quad [3]$$

On the Global Convergence of Gradient Descent for Over-parameterized Models using Optimal Transport

Lénaïc Chizat
INRIA, ENS, PSL Research University
Paris, France
lenaic.chizat@inria.fr

Francis Bach
INRIA, ENS, PSL Research University
Paris, France
francis.bach@inria.fr

Abstract

Many tasks in machine learning and signal processing can be solved by minimizing a convex function of a measure. This includes sparse spikes deconvolution or training a neural network with a single hidden layer. For these problems, we study a simple minimization method: the unknown measure is discretized into a mixture of particles and a continuous-time gradient descent is performed on their weights

Data Model

Data: $\{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_n, y_n)\} \sim_{\text{i.i.d.}} \mathbb{P}(\mathbb{R}^d \times \mathbb{R})$

$$\boldsymbol{x}_i \sim \text{Unif}(\Omega) \text{ and } y_i = f(\boldsymbol{x}_i)$$

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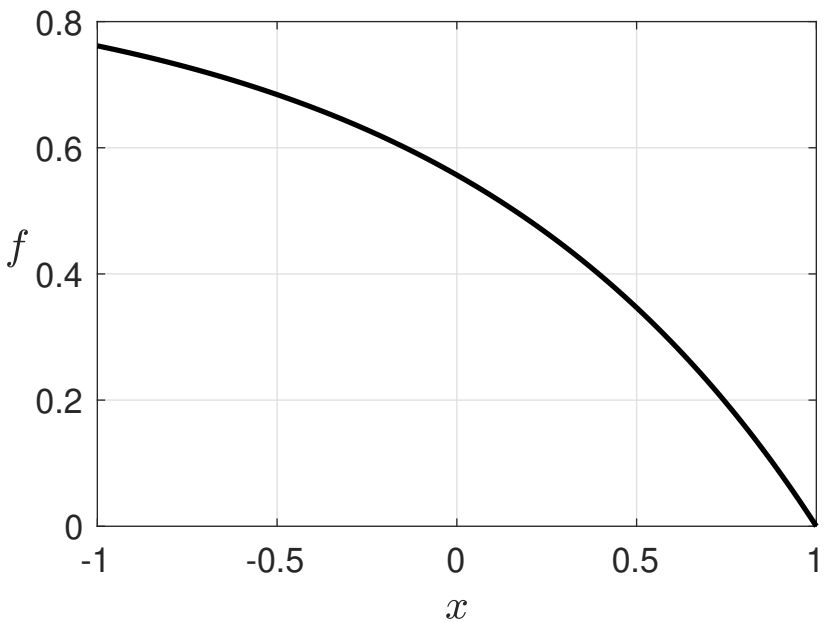
$$\boldsymbol{x}_i \sim \text{Unif}(\Omega) \text{ and } y_i = f(\boldsymbol{x}_i)$$

- Ω bounded and convex
- f positive, smooth and γ-strongly concave



Problem Statement

Goal: Minimize loss $L_N(\boldsymbol{w}) = \mathbb{E}\Big\{\Big(y - \frac{1}{N}\sum_{i=1}^{N}\sigma(\boldsymbol{x};\boldsymbol{w}_i)\Big)^2\Big\}$

Problem Statement

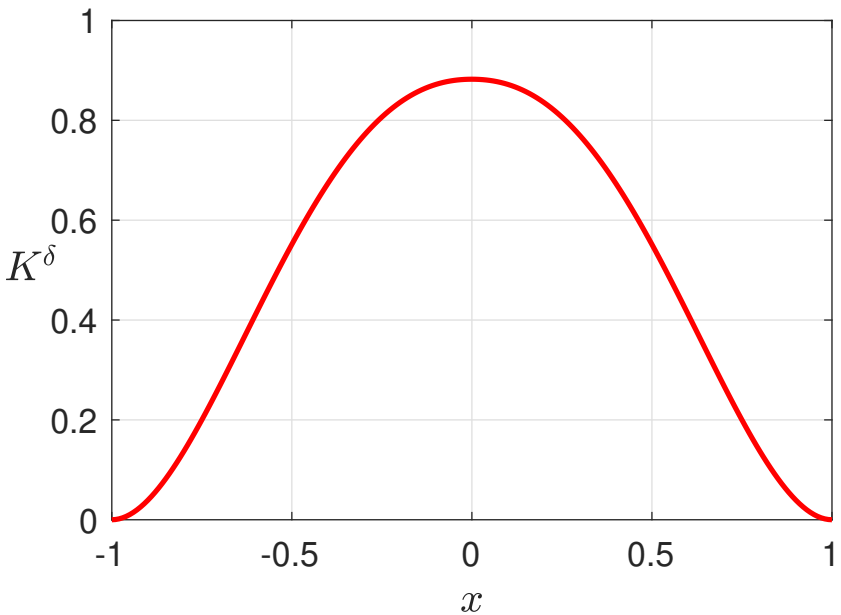
Goal: Minimize loss $L_N(\boldsymbol{w}) = \mathbb{E}\left\{\left(y - \frac{1}{N}\sum_{i=1}^{N}\sigma(\boldsymbol{x};\boldsymbol{w}_i)\right)^2\right\}$

- σ 'bump'-like

$\sigma(\boldsymbol{x};\boldsymbol{w}_i) = K^\delta(\boldsymbol{x} - \boldsymbol{w}_i)$

- $\boldsymbol{w}_i$ = center of bump
- δ = width of the bump

$K^\delta(\boldsymbol{x}) = \delta^{-d}K(\boldsymbol{x}/\delta)$



Exponential and Dimension-free Convergence Rate

Theorem [JMM20]

Let f be γ-strongly concave, σ a bump of width δ, and $\boldsymbol{w}^k$ obtained after k SGD iterations with step size α. Then, with high probability,

$$\underbrace{L_N(\boldsymbol{w}^k)}_{\text{loss at step } k} \leq L_N(\boldsymbol{w}^0) \underbrace{e^{-2\gamma k\alpha}}_{\text{exp. rate}} + \underbrace{\Delta(N,\alpha,\delta)}_{\text{distance to opt.}},$$

where $\Delta(N,\alpha,\delta) \to 0$ as $N \to \infty$, $\alpha \to 0$, and $\delta \to 0$.

- As $\delta \to 0$, gradient flow optimizes a **displacement convex** loss.

[JMM20] A. Javanmard, M. Mondelli, and A. Montanari, "Analysis of a Two-Layer Neural Network via Displacement Convexity", *Annals of Statistics*, 2020+.

Thank You for Your Attention