Global convergence of gradient descent for non-convex learning problems

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Institut Henri Poincaré - April 5, 2019

Machine learning
Scientific context

- **Proliferation of digital data**
  - Personal data
  - Industry
  - Scientific: from bioinformatics to humanities

- **Need for automated processing of massive data**

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- **Healthy interactions between theory, applications, and hype?**

Recent progress in perception (vision, audio, text)

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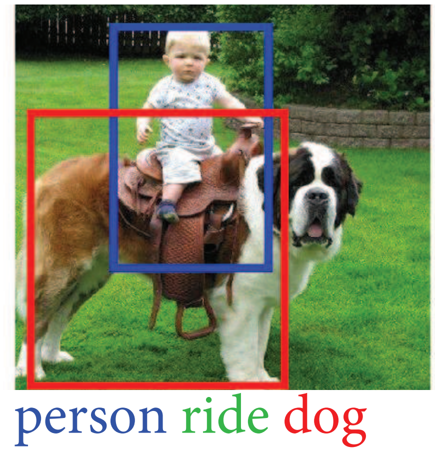

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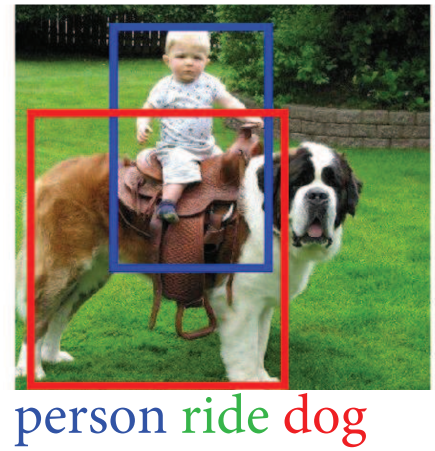

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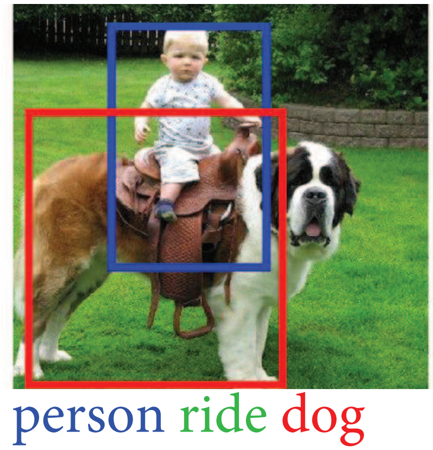

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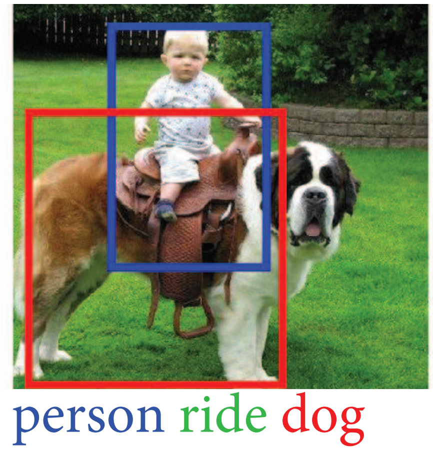

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Parametric supervised machine learning

- **Data**: n observations $(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}$, $i = 1, \dots, n$
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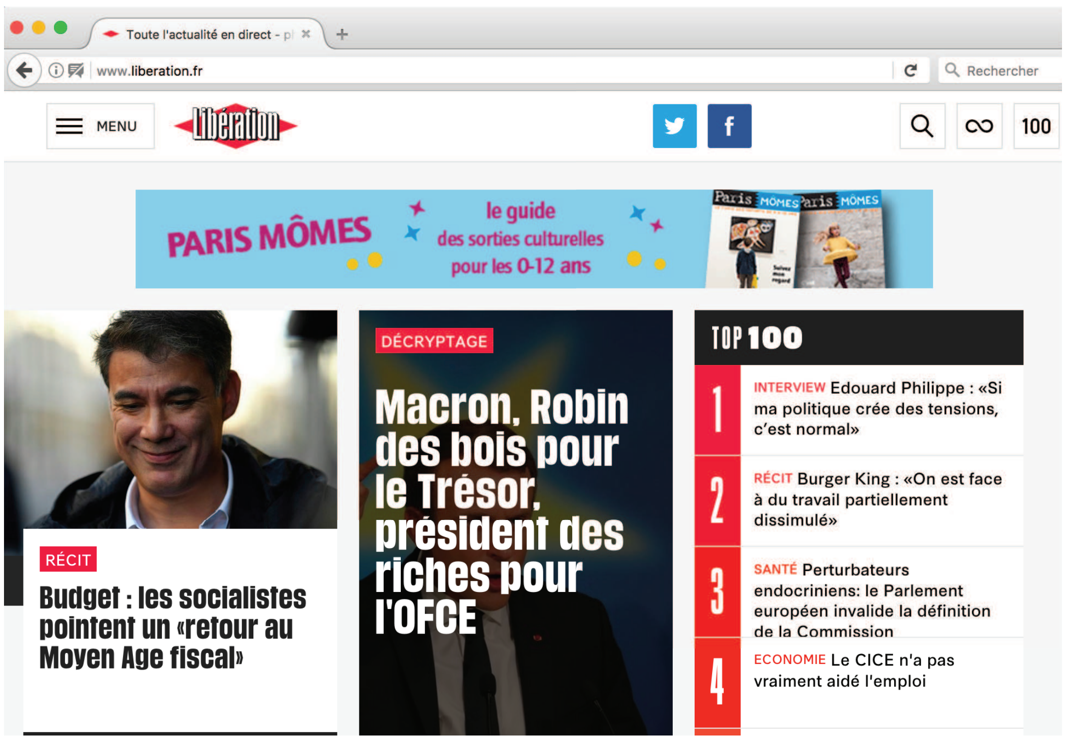

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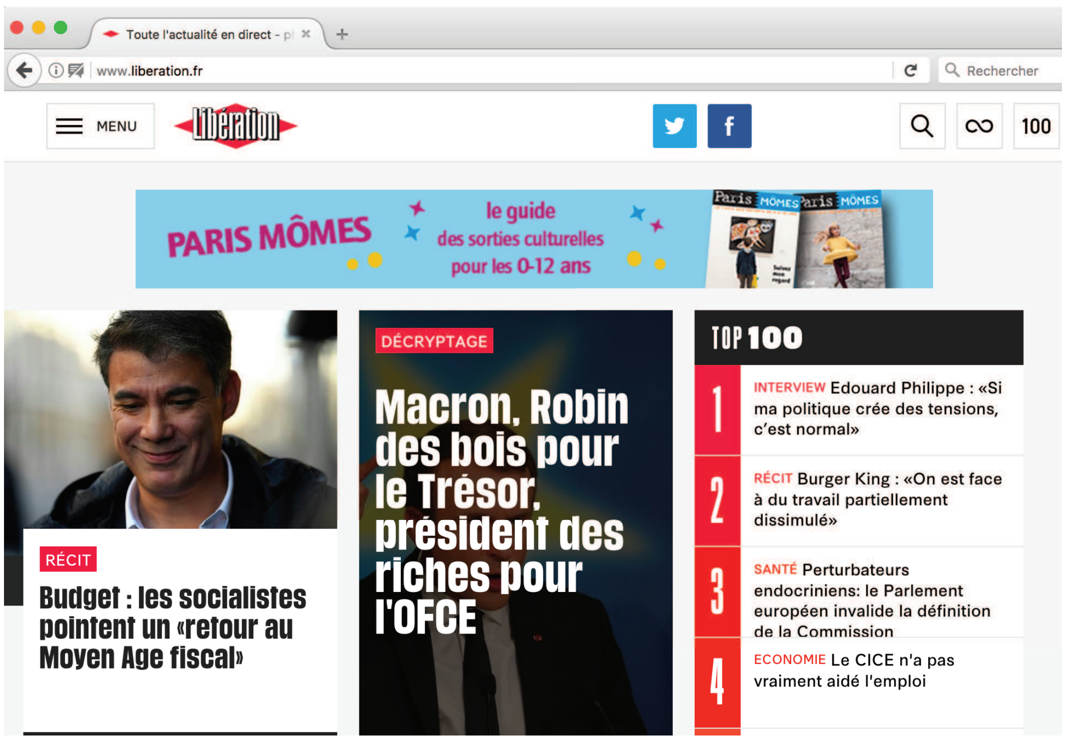

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- Linear predictions
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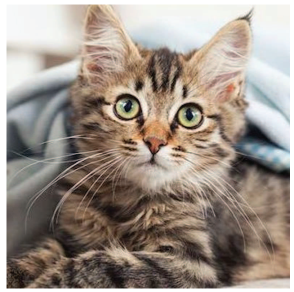
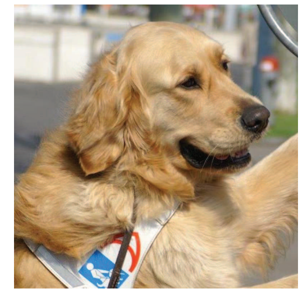
x_1	x_2	x_3	x_4	x_5	x_6
					
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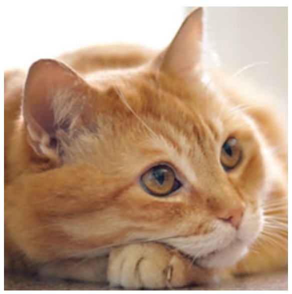

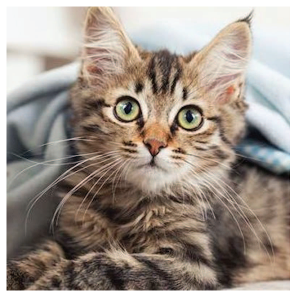
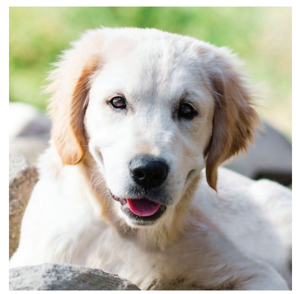

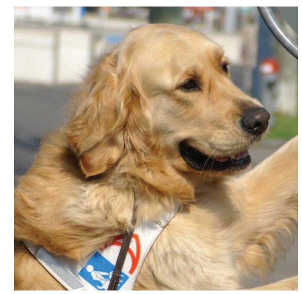

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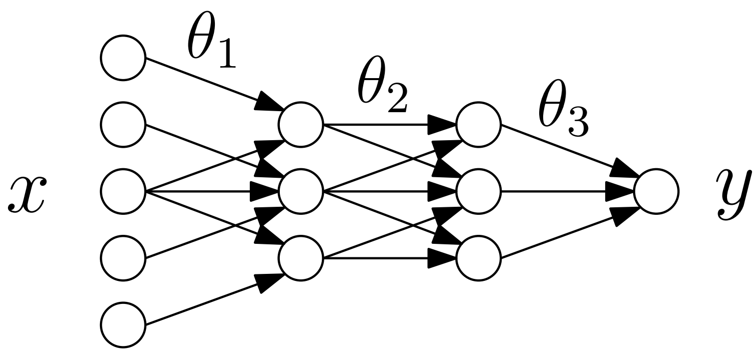

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- **(regularized) empirical risk minimization**:

$$\min_{\theta \in \mathbb{R}^d} \quad \frac{1}{n} \sum_{i=1}^{n} \quad \ell\big(y_i, h(x_i, \theta)\big) \quad + \quad \lambda \Omega(\theta)$$

data fitting term $+$ regularizer

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- **Actual goal**: minimize test error $\mathbb{E}_{p(x,y)} \ell(y, h(x, \theta))$

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- **Golden years of convexity in machine learning** (1995 to 201*)
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  - Sparsity / low-rank models with first-order methods
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Exponentially convergent SGD for smooth finite sums

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  - SAG (Le Roux, Schmidt, and Bach, 2012)
  - SDCA (Shalev-Shwartz and Zhang, 2013)
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  - MISO (Mairal, 2015), Finito (Defazio et al., 2014a)
  - SAGA (Defazio, Bach, and Lacoste-Julien, 2014b), etc...

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- **Accelerated algorithms**
  - Shalev-Shwartz and Zhang (2014); Nitanda (2014)
  - Lin et al. (2015b); Defazio (2016), etc...
  - Catalyst (Lin, Mairal, and Harchaoui, 2015a)

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- **Running-time to reach precision** ε (with $\kappa =$ condition number)

Gradient descent	$d\times$	$n\kappa$	$\times \log \frac{1}{\varepsilon}$
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NB: slightly different (smaller) notion of condition number for batch methods

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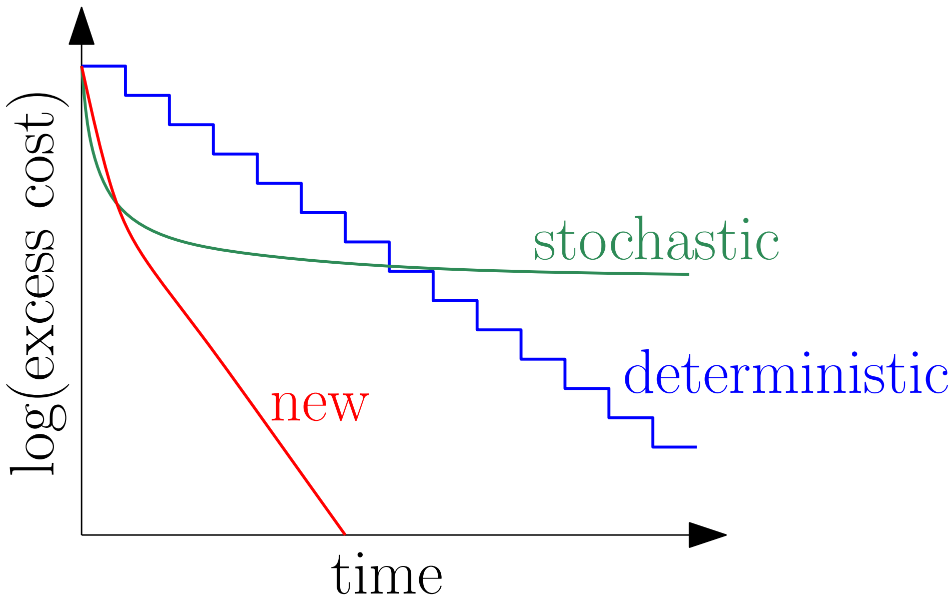
- **Beating two lower bounds** (Nemirovski and Yudin, 1983; Nesterov, 2004): with additional assumptions

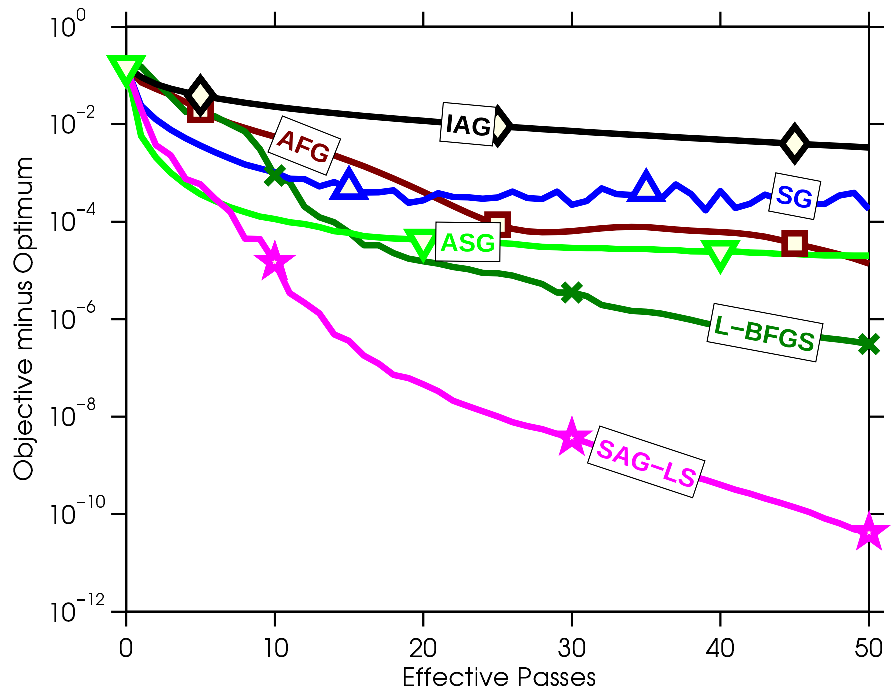
(1) stochastic gradient: exponential rate for finite sums

(2) full gradient: better exponential rate using the sum structure

- **Matching lower bounds** (Woodworth and Srebro, 2016; Lan, 2015)

Exponentially convergent SGD for finite sums
From theory to practice and vice-versa





- **Empirical performance “matches” theoretical guarantees**

- **Theoretical analysis suggests practical improvements**
  - Non-uniform sampling, acceleration
  - Matching upper and lower bounds

Convex optimization for machine learning
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  - Non-parametric and high-dimensional regression
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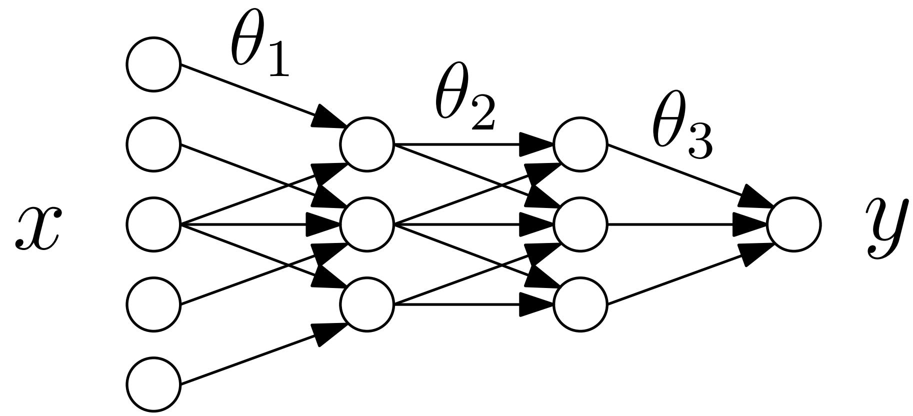
- **What about deep learning?**

Theoretical analysis of deep learning

- **Multi-layer neural network** $h(x,\theta) = \theta_m^\top \sigma(\theta_{m-1}^\top \sigma(\cdots \theta_2^\top \sigma(\theta_1^\top x))$



  – NB: already a simplification

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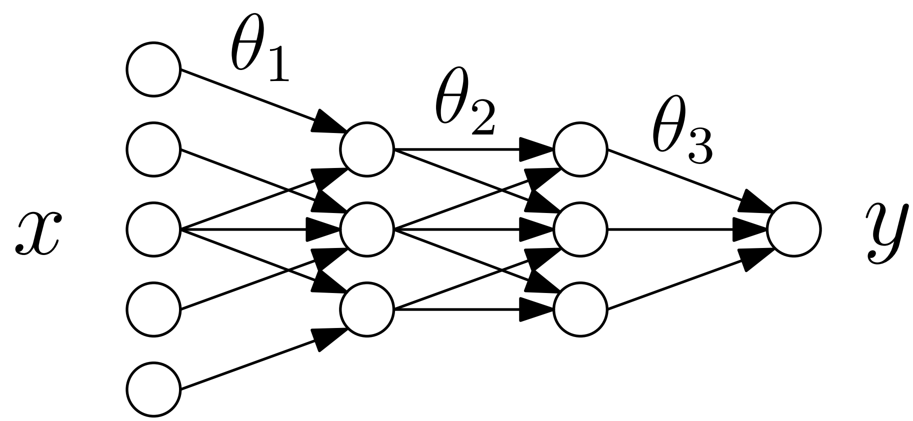

- **Generalization guarantees**
  - See "MythBusters: A Deep Learning Edition" by Sasha Rakhlin
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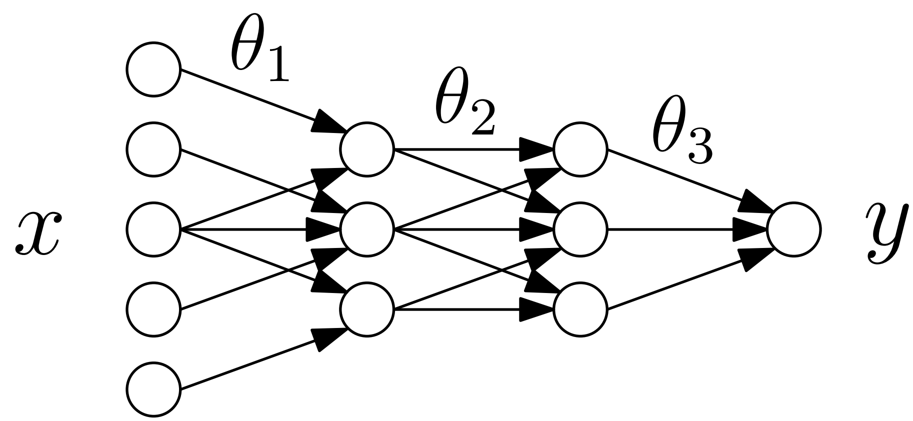

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- **Optimization**
  - Non-convex optimization problems

Optimization for multi-layer neural networks

- **What can go wrong with non-convex optimization problems?**
  - Local minima
  - Stationary points
  - Plateaux
  - Bad initialization
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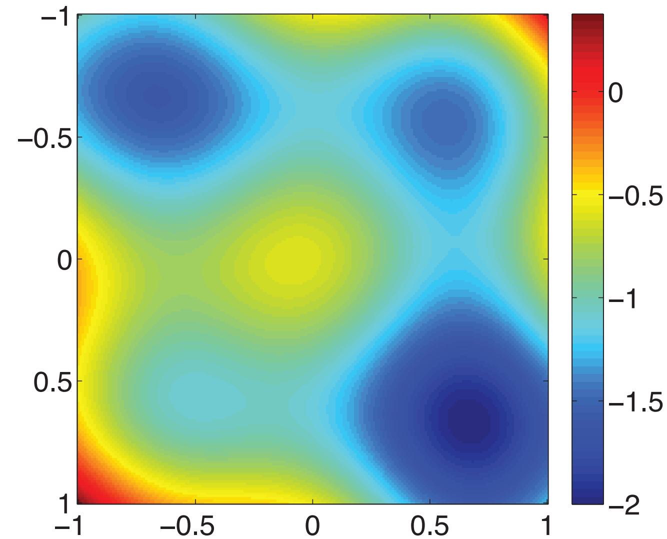

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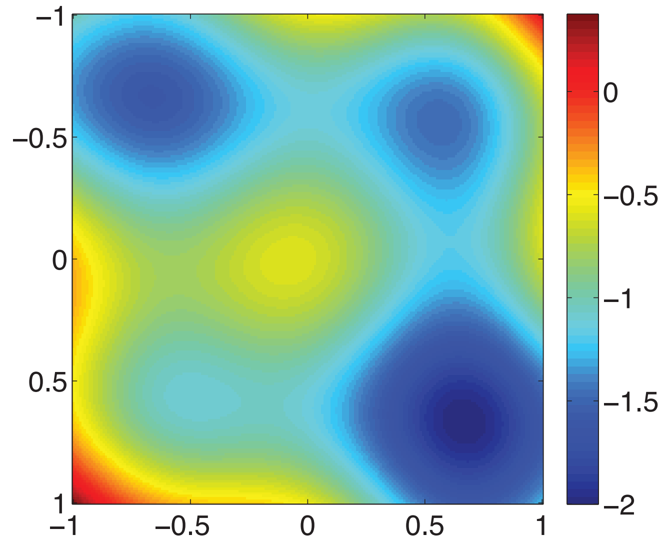

- **Generic local theoretical guarantees**
  - Convergence to stationary points or local minima
  - See, e.g., Lee et al. (2016); Jin et al. (2017)

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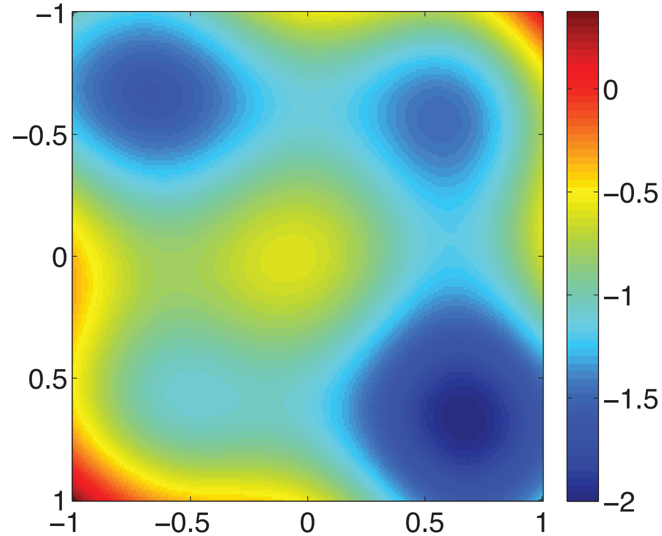

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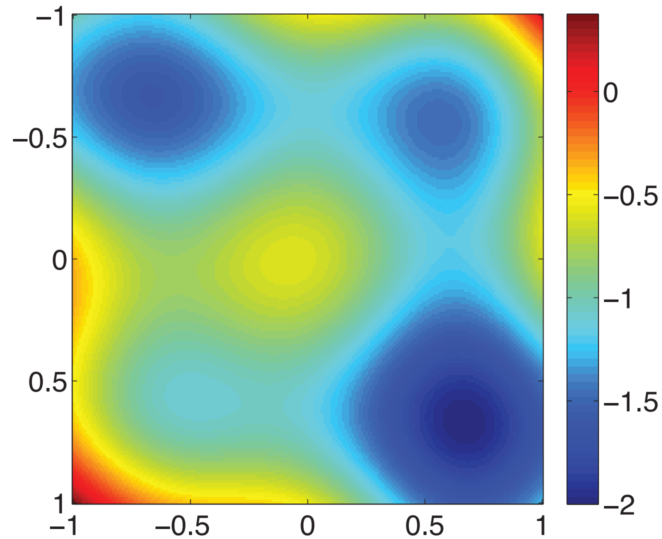

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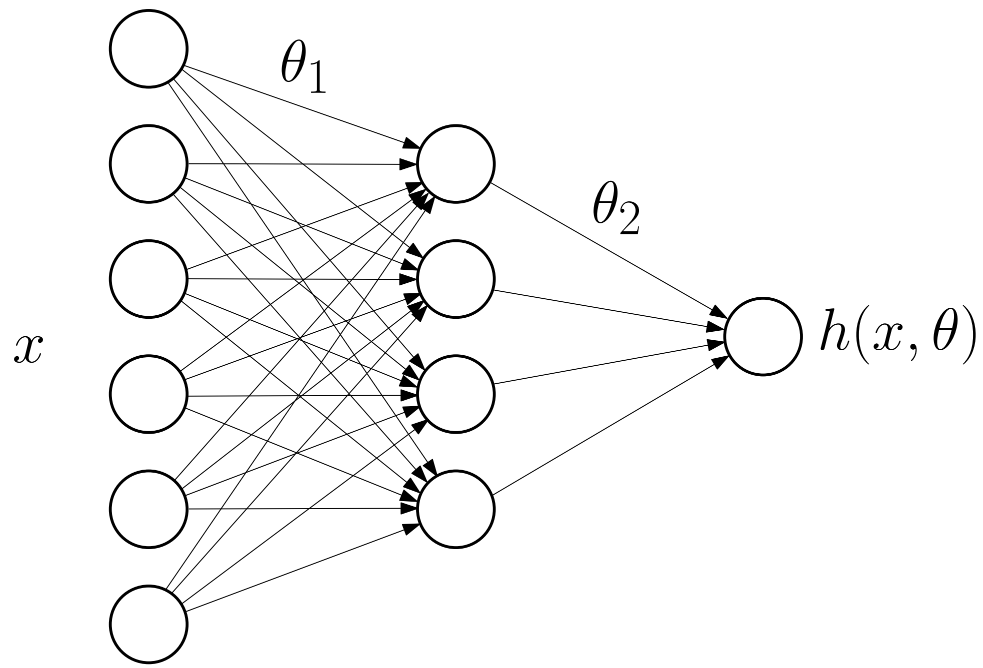
- **Special case of (deep) neural networks**
  – Most local minima are equivalent (Choromanska et al., 2015)
  – No spurrious local minima (Soltanolkotabi et al., 2018)
  – NB: see Jain and Kar (2017) for guarantees in other contexts

Gradient descent for a single hidden layer

- **Predictor**: $h(x) = \theta_2^\top \sigma(\theta_1^\top x) = \sum_{i=1}^m \theta_2(i) \cdot \sigma\big[\theta_1(\cdot, i)^\top x\big]$

- **Goal**: minimize $R(h) = \mathbb{E}_{p(x,y)} \ell(y, h(x))$, with R convex



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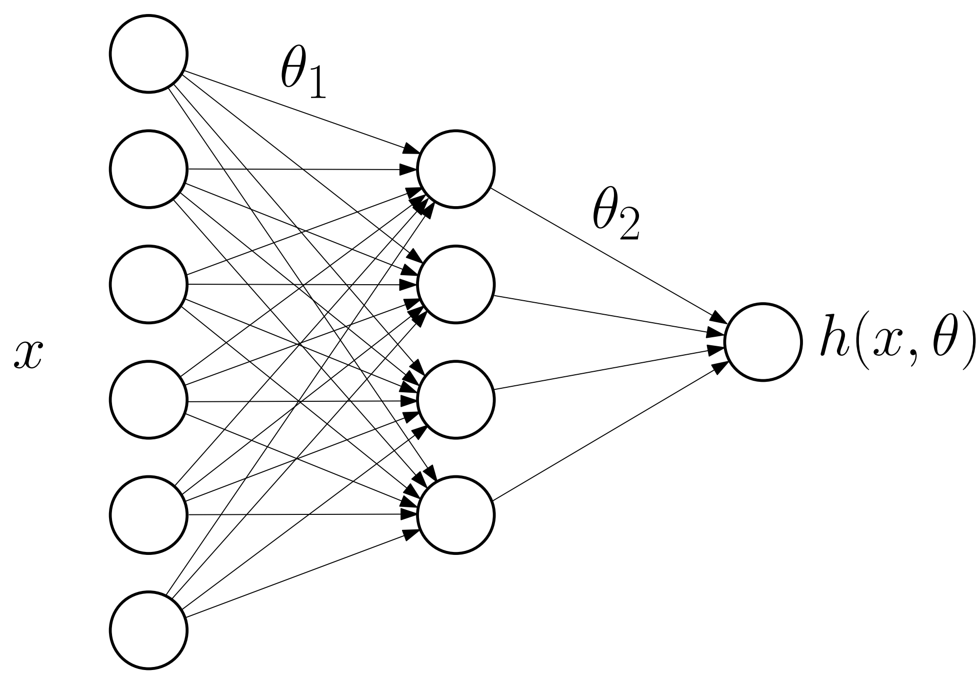

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- **Goal**: minimize $R(h) = \mathbb{E}_{p(x,y)} \ell(y, h(x))$, with R convex
- **Main insight**
  - $h = \dfrac{1}{m}\displaystyle\sum_{i=1}^m \Psi(w_i) = \int_{\mathcal{W}} \Psi(w) d\mu(w)$ with $d\mu(w) = \dfrac{1}{m}\displaystyle\sum_{i=1}^m \delta_{w_i}$
  - Overparameterized models with m large $\approx$ measure μ with densities
  - Barron (1993); Kurkova and Sanguineti (2001); Bengio et al. (2006); Rosset et al. (2007); Bach (2014)

Optimization on measures

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- **Represent** μ **by a finite set of "particles"** $\mu = \frac{1}{m}\sum_{i=1}^{m} \delta_{w_i}$
  - Backpropagation $=$ gradient descent on $(w_1, \dots, w_m)$

- **Two questions**:
  - Algorithm limit when number of particles m gets large

  - Global convergence

Optimization on measures

- **Minimize with respect to measure** μ: $R\Big(\int_{\mathcal{W}} \Psi(w) d\mu(w)\Big)$
  - Convex optimization problem on measures
  - Frank-Wolfe techniques for incremental learning
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- **Two questions**:
  - Algorithm limit when number of particles m gets large
    Wasserstein gradient flow (Nitanda and Suzuki, 2017)
  - Global convergence
    to the optimal measure μ (Chizat and Bach, 2018a)

Many particle limit and global convergence (Chizat and Bach, 2018a)

- **General framework**: minimize $F(\mu) = R\Big(\int_{\mathcal{W}} \Psi(w) d\mu(w) \Big)$
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- **Limit when m tends to infinity**

  – Wasserstein gradient flow (Nitanda and Suzuki, 2017; Chizat and Bach, 2018a; Mei, Montanari, and Nguyen, 2018; Sirignano and Spiliopoulos, 2018; Rotskoff and Vanden-Eijnden, 2018)

- NB: for more details on gradient flows, see Ambrosio et al. (2008)

(intuitive) link with Wasserstein gradient flows

- Gradient flow on Euclidean spaces, for smooth function $f : \mathcal{A} \to \mathbb{R}$
  - Given $a = a(t)$, $a(t + dt)$ is the minimizer of $f(b) + \dfrac{1}{2dt}\|b - a\|^2$
  - Optimality conditions: $\nabla f(b) + \dfrac{1}{dt}(b - a) = 0$

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  - For smooth f, $\nabla f(b) - \nabla f(a) = O(dt)$
  - Thus $a(t + dt) = b = a - (dt)\nabla f(a) = a(t) - (dt)\nabla f(a(t))$
  - Equivalent to regular ODE: $\dot{a} = -\nabla f(a)$

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- Given measure $\mu = \mu(t)$, $\nu = \mu(t + dt)$ defined as the minimizer of

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  - $\Pi(\mu,\nu)$ set of joint distributions with marginals μ and ν

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- **Global convergence ?**
  - Difficulty 1: potentially many local minima and stationary points (even if R is convex)
  - Difficulty 2: globally optimal measure is often singular

Many particle limit and global convergence (Chizat and Bach, 2018a)

- **Two ingredients**: homogeneity and initialization

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- **Homogeneity** (see, e.g., Haeffele and Vidal, 2017; Bach et al., 2008)
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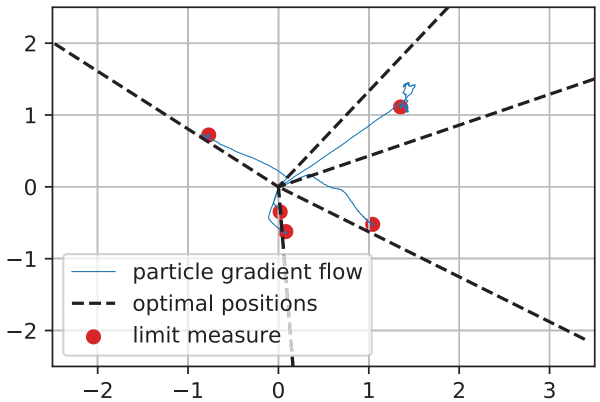
- NB 1 : see precise definitions and statement in paper

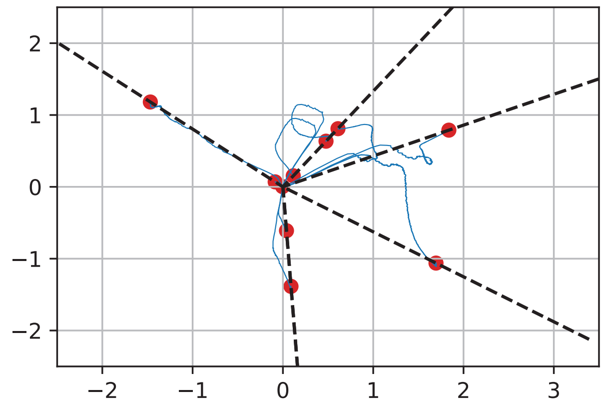
- NB 2 : also applies to spike deconvolution

Simple simulations with neural networks

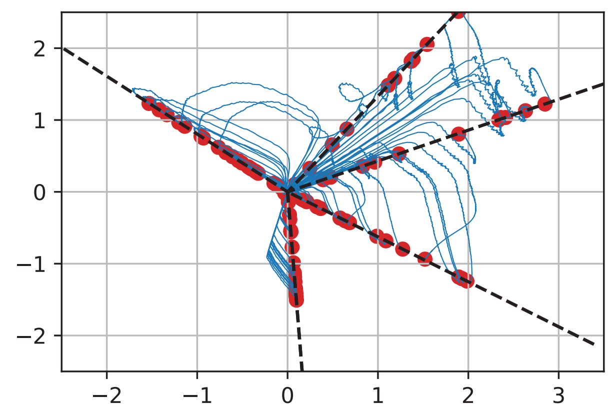
- ReLU units with $d = 2$ (optimal predictor has 5 neurons)



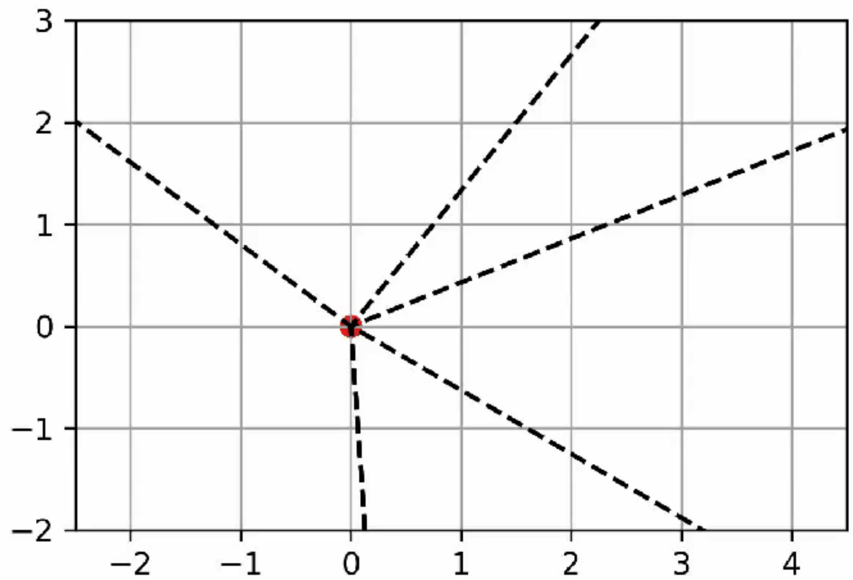
5 neurons



10 neurons

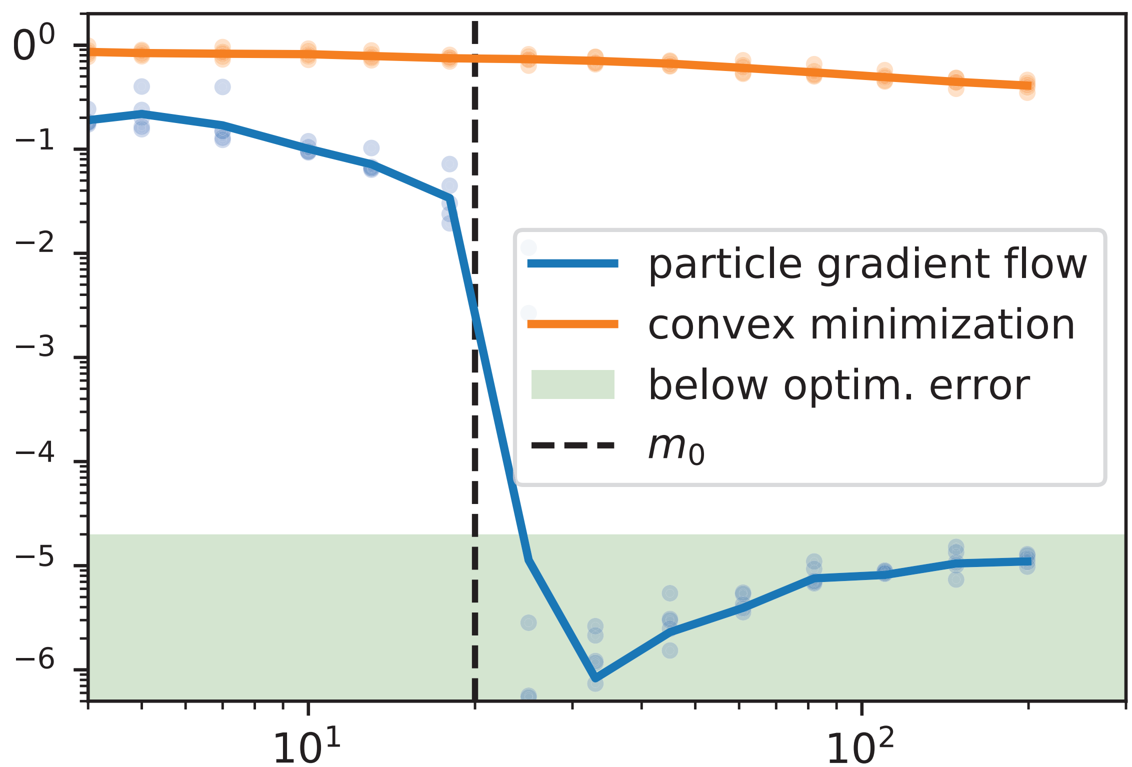


100 neurons



Simple simulations with neural networks

- ReLU units with $d = 100$ (optimal predictor has m_0 neurons)
  - Comparing gradient descent on particles with sampling (and reweighting by convex optimization) fixed particles
  - No quantitative analysis (yet)



From qualitative to quantitative results ?

- **Adding noise** (Mei, Montanari, and Nguyen, 2018)
  - On top of SGD "à la Langevin" $\Rightarrow$ convergence to a diffusion
  - Quantitative analysis of the needed number of neurons
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- **Recent strong activity on ArXiv**
  - `https://arxiv.org/abs/1810.02054`
  - `https://arxiv.org/abs/1811.03804`
  - `https://arxiv.org/abs/1811.03962`
  - `https://arxiv.org/abs/1811.04918`
  - See also Jacot et al. (2018)

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- **Recent strong activity on ArXiv**
  - Global quantitative linear convergence of gradient descent
  - Zero training loss
  - Extends to deep architectures and skip connections

From qualitative to quantitative results ?

- **Mean-field limit**: $h(x) = \frac{1}{m}\sum_{i=1}^{m} \Psi(w_i)$
  - With w_i initialized randomly (with variance independent of m)
  - Dynamics equivalent to Wasserstein gradient flow
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- **Equivalence to lazy training** (Chizat and Bach, 2018b)
  - Convergence to a positive-definite kernel method
  - Neurons move infinitesimally

Lazy training (Chizat and Bach, 2018b)

- **Generic criterion** $G(W) = R(h(W))$ **to minimize w.r.t.** W
  - Example: R loss, $h = \frac{1}{m}\sum_{i=1}^{m} \Psi(w_i)$ prediction function
  - Introduce (large) scale factor $\alpha > 0$ and $G_\alpha(W) = G(\alpha h(W))/\alpha^2$
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    (using e.g., $\mathbb{E}\Psi(w_i) = 0$)

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- **Proposition** (informal)
  - Assume differential of h at $W(0)$ is surjective
  - Gradient flow $\dot{W} = -\nabla G_\alpha(W)$ is such that

    $\|W(t) - W(0)\| = O(1/\alpha)$ and $\alpha h(W(t)) \to \arg\min_h R(h)$ "linearly"

$\Rightarrow$ Equivalent to a linear model
$h(W) \approx h(W(0)) + (W - W(0))^\top \nabla h(W(0))$

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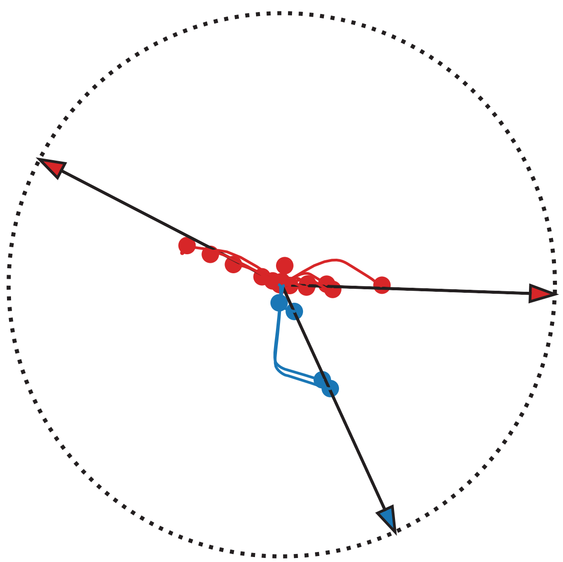

Lazy
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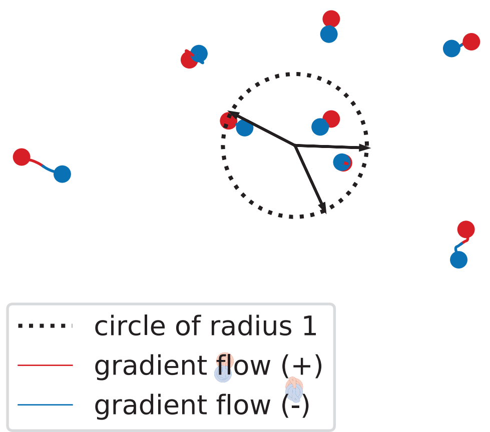

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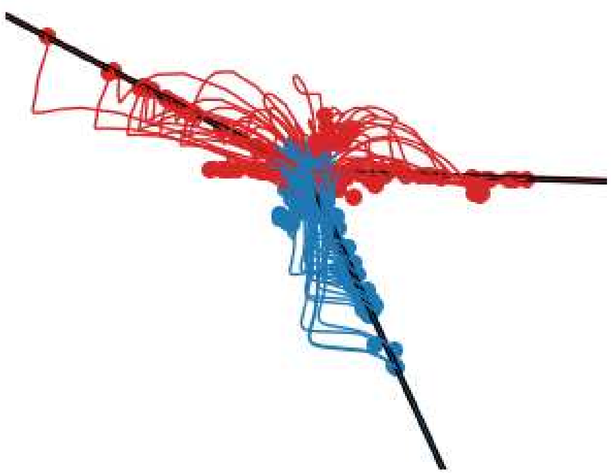

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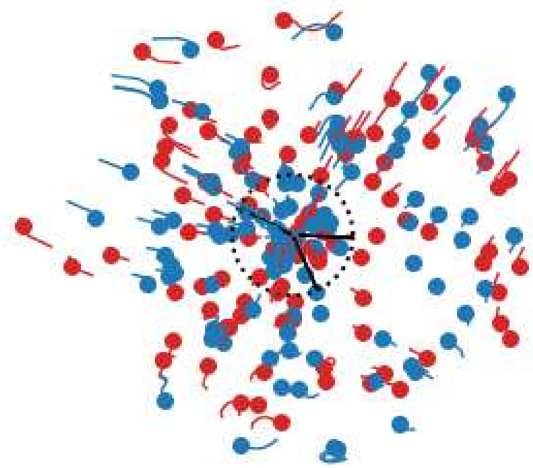

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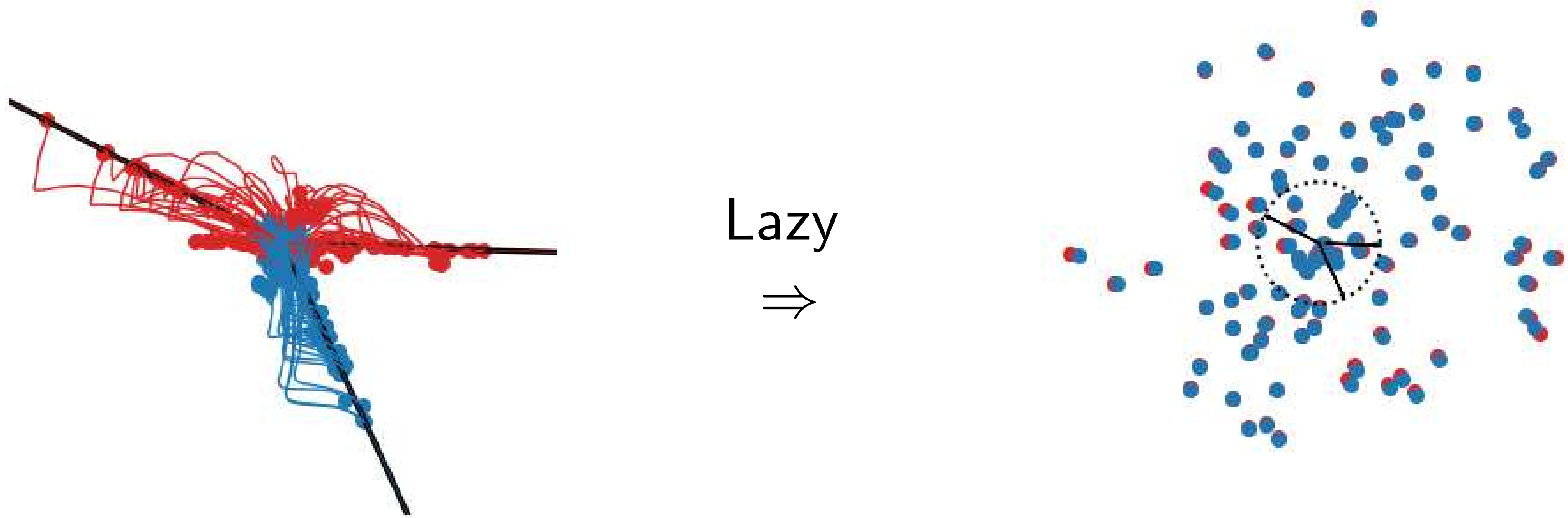

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  - Still non-parametric estimation
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- **What is actually happening in practice?** (ongoing work)
  - Between mean field regime and lazy regime?
  - Empirical comparison for state-of-the-art networks

Healthy interactions between theory, applications, and hype?

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Healthy interactions between theory, applications, and hype?

- **Empirical successes of deep learning cannot be ignored**
- **Scientific standards should not be lowered**
  - Critics and limits of theoretical and empirical results
  - Rigor beyond mathematical guarantees

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