Optimization for Machine Learning
From Convex to Non-convex

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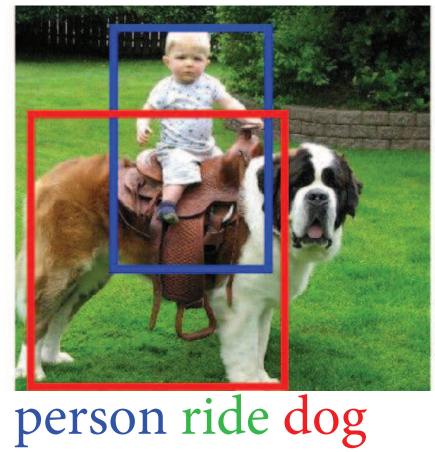
Scientific context

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

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

Recent progress in perception (vision, audio, text)

From translate.google.fr



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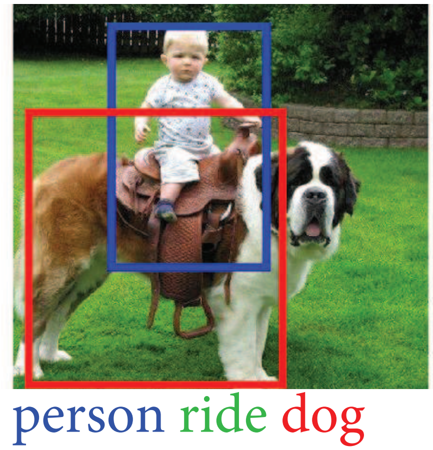

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(1) **Massive data**

(2) **Computing power**

(3) **Methodological and scientific progress**

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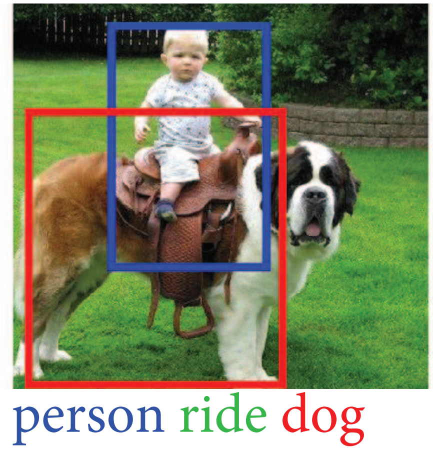

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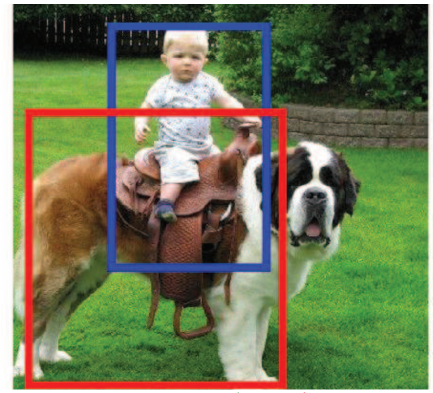

person ride dog

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Parametric supervised machine learning

- **Data**: n observations $(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}$, $i = 1, \dots, n$
- **Prediction function** $h(x, \theta) \in \mathbb{R}$ parameterized by $\theta \in \mathbb{R}^d$

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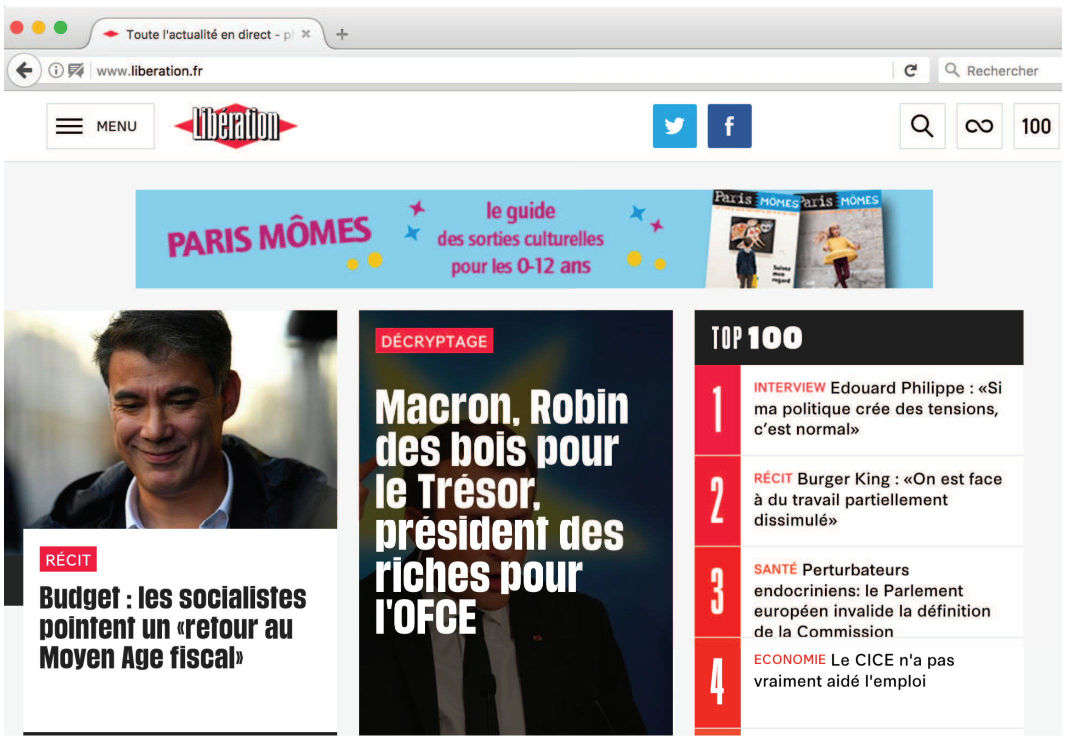

- Linear predictions
  - $h(x, \theta) = \theta^\top \Phi(x)$
- E.g., **advertising**: $n > 10^9$
  - $\Phi(x) \in \{0, 1\}^d$, $d > 10^9$
  - Navigation history + ad

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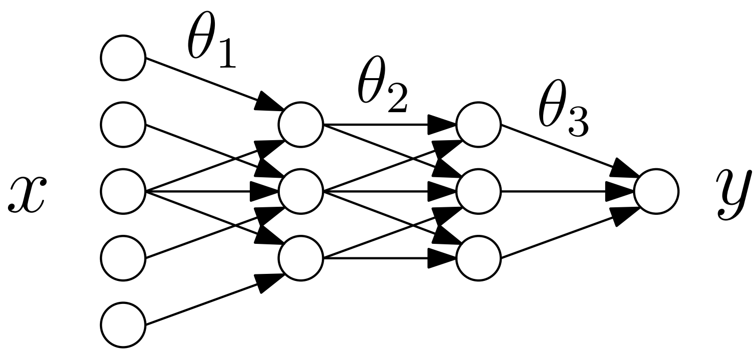
x_1 x_2 x_3 x_4 x_5 x_6

$y_1 = 1$ $y_2 = 1$ $y_3 = 1$ $y_4 = -1$ $y_5 = -1$ $y_6 = -1$

  – Neural networks $(n, d > 10^6)$: $h(x, \theta) = \theta_r^\top \sigma(\theta_{r-1}^\top \sigma(\cdots \theta_2^\top \sigma(\theta_1^\top x))$



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- **Prediction function** $h(x, \theta) \in \mathbb{R}$ parameterized by $\theta \in \mathbb{R}^d$
- **(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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data fitting term + regularizer

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

Convex optimization problems

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

- **Conditions**: Convex loss and linear predictions $h(x, \theta) = \theta^\top \Phi(x)$

- **Consequences**
  - Efficient algorithms (typically gradient-based)
  - Quantitative runtime and prediction performance guarantees

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- **Golden years of convexity in machine learning** (1995 to 2020)
  - Support vector machines and kernel methods
  - Sparsity / low-rank models with first-order methods
  - Optimal transport
  - Stochastic methods for large-scale learning and online learning
  - etc.

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Exponentially convergent SGD for smooth finite sums

- **Finite sums**: $\displaystyle \min_{\theta \in \mathbb{R}^d} \quad \frac{1}{n} \sum_{i=1}^{n} f_i(\theta) = \frac{1}{n} \sum_{i=1}^{n} \Big\{ \ell\big(y_i, h(x_i, \theta)\big) + \lambda \Omega(\theta) \Big\}$

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- **Non-accelerated algorithms** (with similar properties)
  - SAG (Le Roux, Schmidt, and Bach, 2012)
  - SDCA (Shalev-Shwartz and Zhang, 2013)
  - SVRG (Johnson and Zhang, 2013; Zhang et al., 2013)
  - SAGA (Defazio, Bach, and Lacoste-Julien, 2014), etc...

$$\theta_t = \theta_{t-1} - \gamma \Big[\nabla f_{i(t)}(\theta_{t-1}) \qquad\qquad\qquad\qquad \Big]$$

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

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- **Running-time to reach precision** ε (with κ = condition number)

Stochastic gradient descent	$d\times$	κ	$\times$	$\frac{1}{\varepsilon}$
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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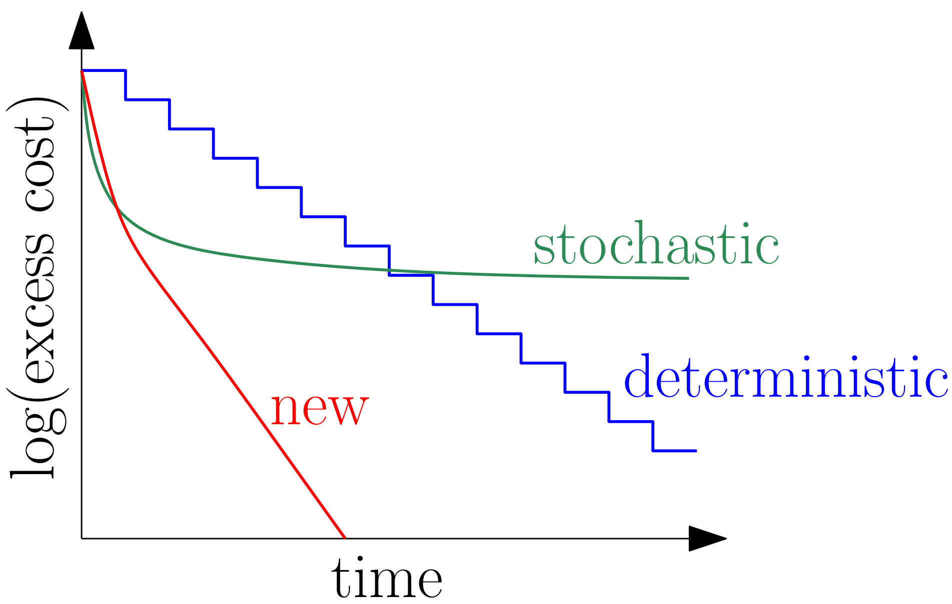
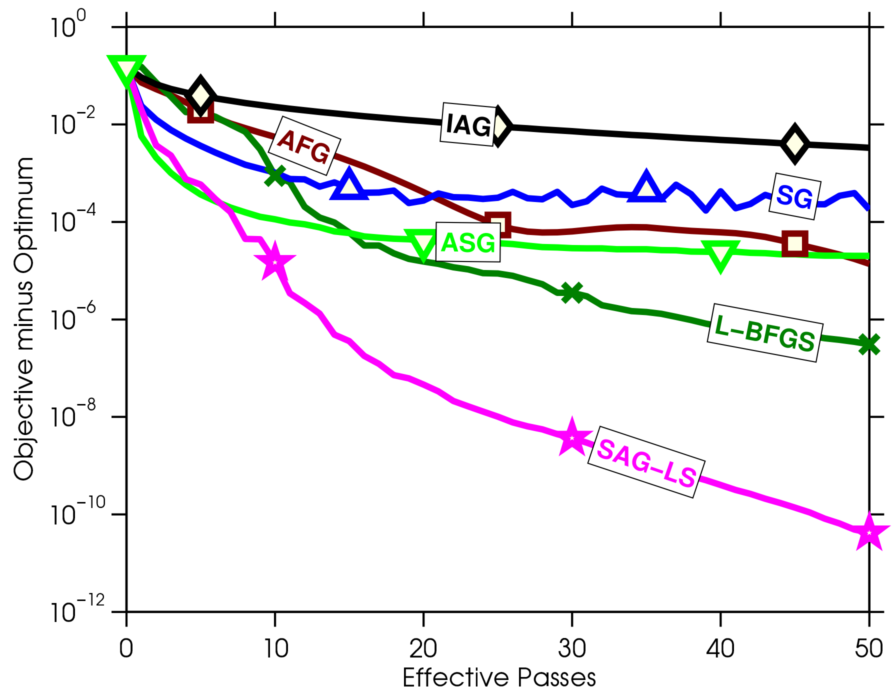
- **Matching lower bounds** (Woodworth and Srebro, 2016; Lan, 2015)

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
From theory to practice and vice-versa

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- **Many other well-understood areas**
  - Single pass SGD and generalization errors
  - Non-parametric and high-dimensional regression
  - Randomized linear algebra
  - Bandit problems
  - etc...

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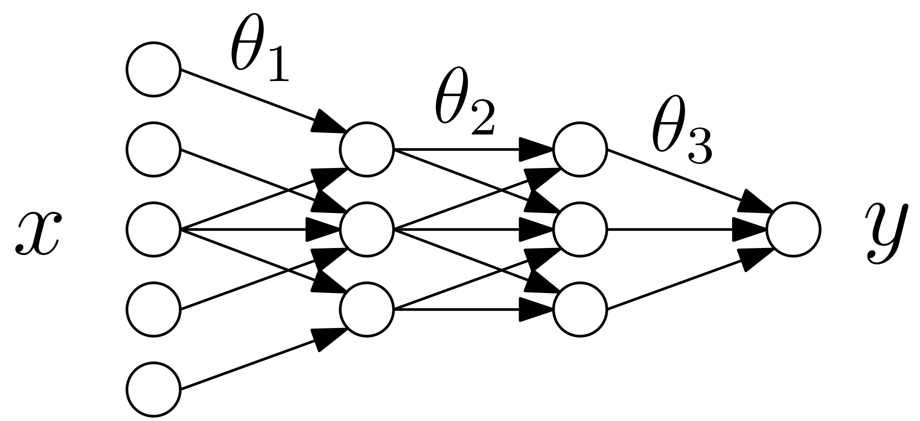
- **What about deep learning?**

Theoretical analysis of deep learning

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



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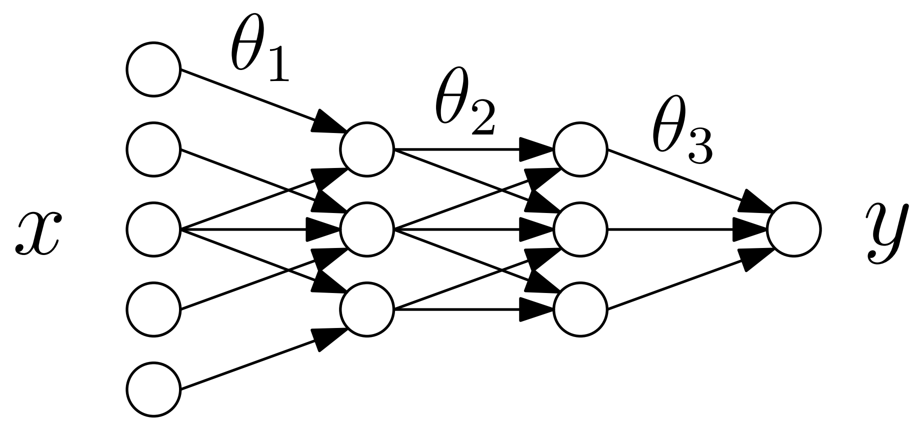

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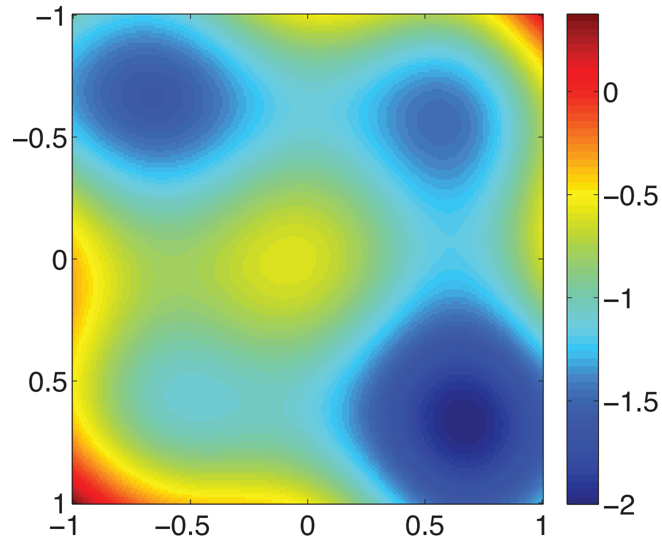
- **Main difficulties**

  1. Non-convex optimization problems

  2. Generalization guarantees in the overparameterized regime

Optimization for multi-layer neural networks

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



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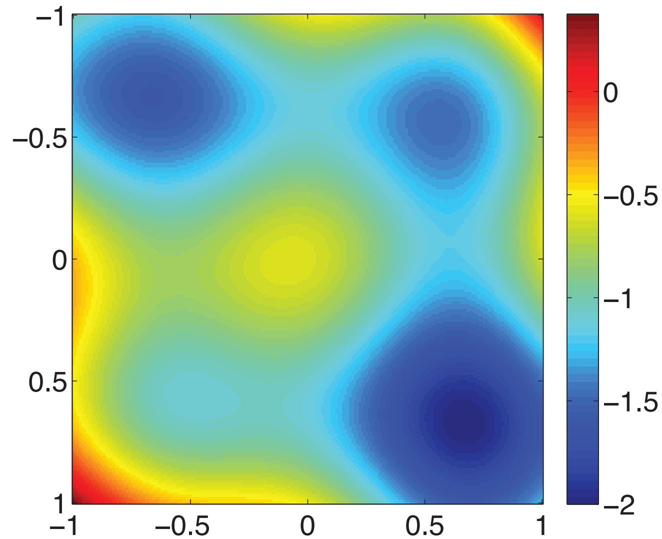

- **Generic local theoretical guarantees**
  - Convergence to stationary points or local minima
  - See, e.g., Lee et al. (2016); Jin et al. (2017)

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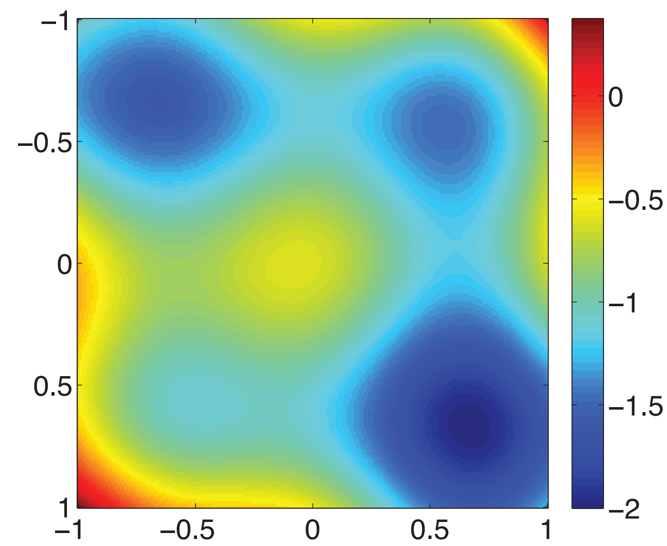

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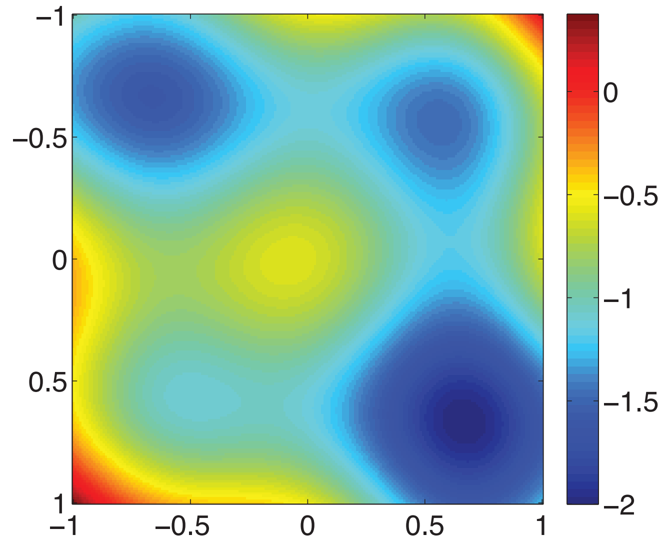

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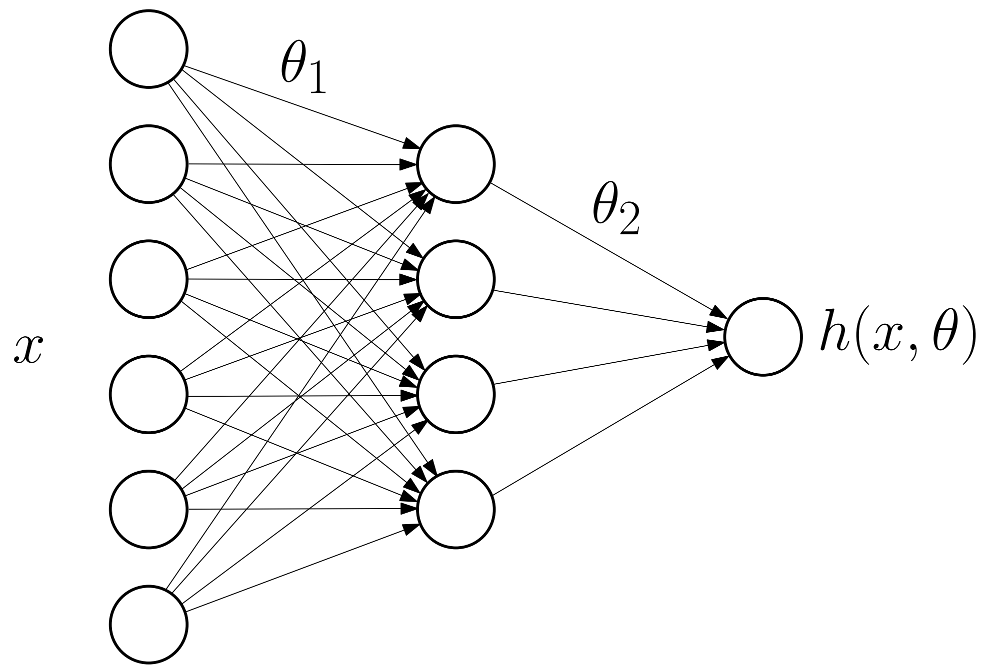
- **Special case of (deep) neural networks**
  - Most local minima are equivalent (Choromanska et al., 2015)
  - No spurrious local minima (Soltanolkotabi et al., 2018)

Gradient descent for a single hidden layer

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

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



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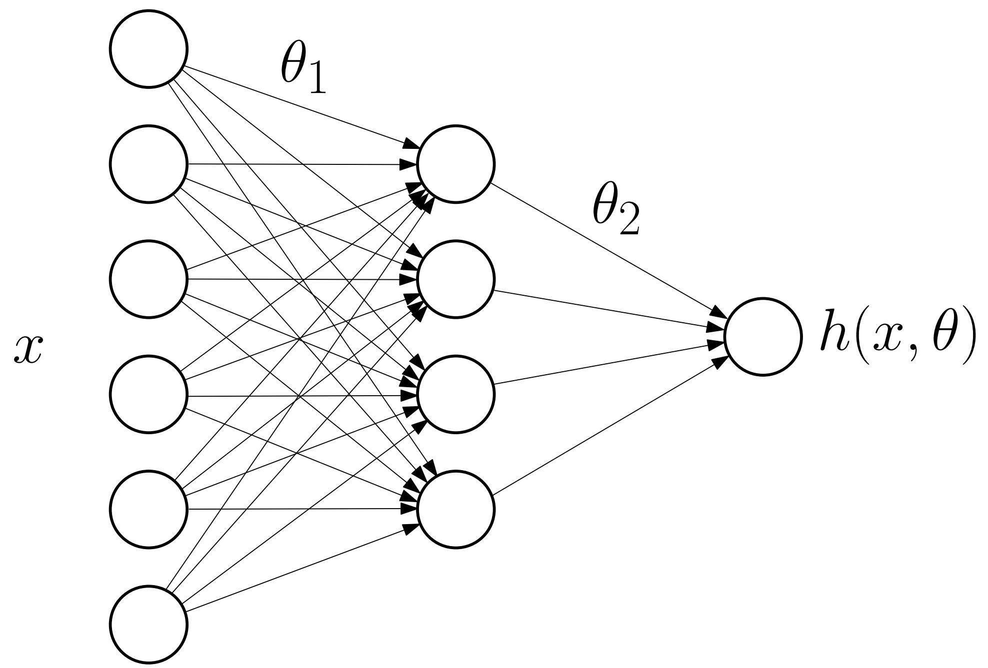

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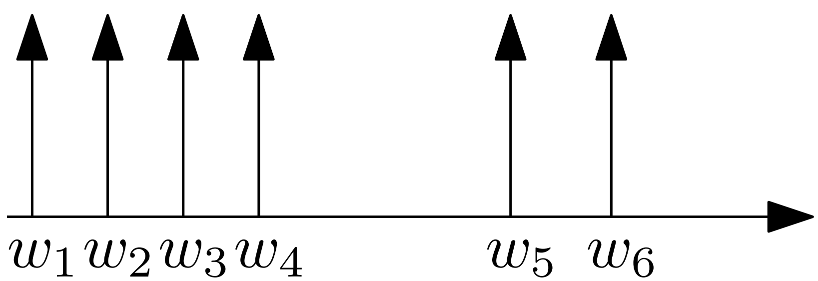
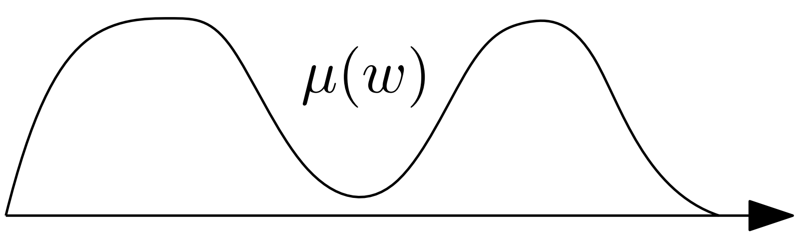
- **Main insight**
  - $h = \displaystyle\frac{1}{m}\sum_{j=1}^m \Psi(w_j) = \int_{\mathcal{W}} \Psi(w) d\mu(w)$ with $d\mu(w) = \displaystyle\frac{1}{m}\sum_{j=1}^m \delta_{w_j}$





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  - 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 (2017)

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
  - Non-tractable (Bach, 2017), not what is used in practice

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  - Non-tractable (Bach, 2017), not what is used in practice
- **Represent** μ **by a finite set of "particles"** $\mu = \frac{1}{m}\sum_{j=1}^{m} \delta_{w_j}$
  - Backpropagation = gradient descent on $(w_1, \dots, w_m)$
- **Three questions**:
  - Algorithm limit when number of particles m gets large
  - Global convergence to a global minimizer
  - Prediction performance

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

- **General framework**: minimize $F(\mu) = R\Big(\int_{\mathcal{W}} \Psi(w) d\mu(w) \Big)$
  - Algorithm: minimizing $F_m(w_1, \dots, w_m) = R\Big(\frac{1}{m} \sum_{j=1}^{m} \Psi(w_j) \Big)$

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  - Gradient flow $\dot{W} = -m \nabla F_m(W)$, with $W = (w_1, \dots, w_m)$
  - Idealization of (stochastic) gradient descent

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  - Idealization of (stochastic) gradient descent
    1. Single pass SGD on the unobserved expected risk
    2. Multiple pass SGD or full GD on the empirical risk

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- **Limit when m tends to infinity**
  - Wasserstein gradient flow (Nitanda and Suzuki, 2017; Chizat and Bach, 2018; Song, 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)

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

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- **Homogeneity** (see, e.g., Haeffele and Vidal, 2017; Bach et al., 2008)
  - Full or partial, e.g., $\Psi(w_j)(x) = m\theta_2(j) \cdot \sigma\big[\theta_1(\cdot, j)^\top x\big]$
  - Applies to rectified linear units (but also to sigmoid activations)
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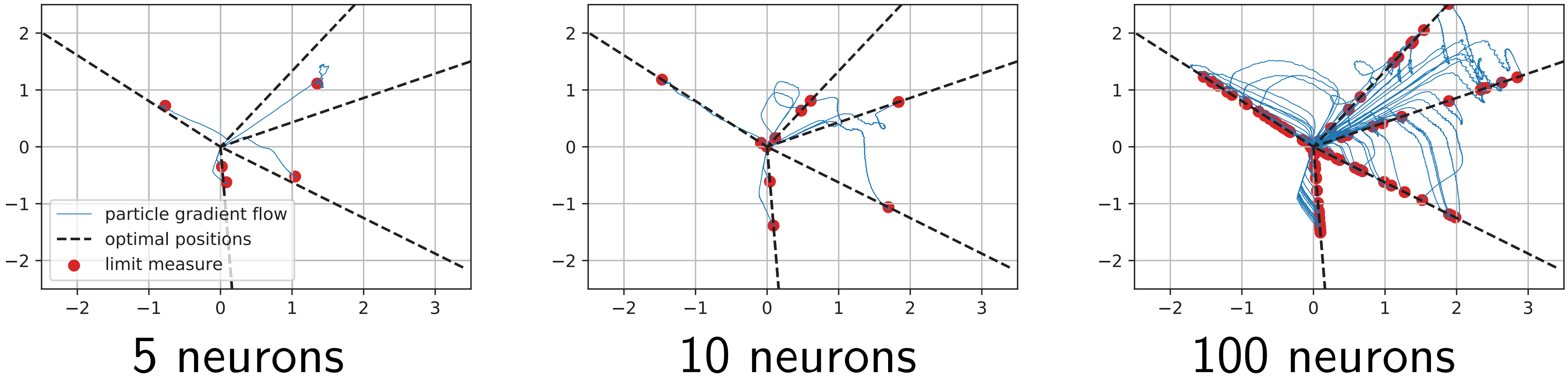
Simple simulations with neural networks

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



$$h(x) = \frac{1}{m} \sum_{j=1}^{m} \Psi(w_j)(x) = \frac{1}{m} \sum_{j=1}^{m} \theta_2(j) \big(\theta_1(\cdot, j)^\top x\big)_+$$

(plotting $|\theta_2(j)|\theta_1(\cdot, j)$ for each hidden neuron j)

NB : also applies to spike deconvolution

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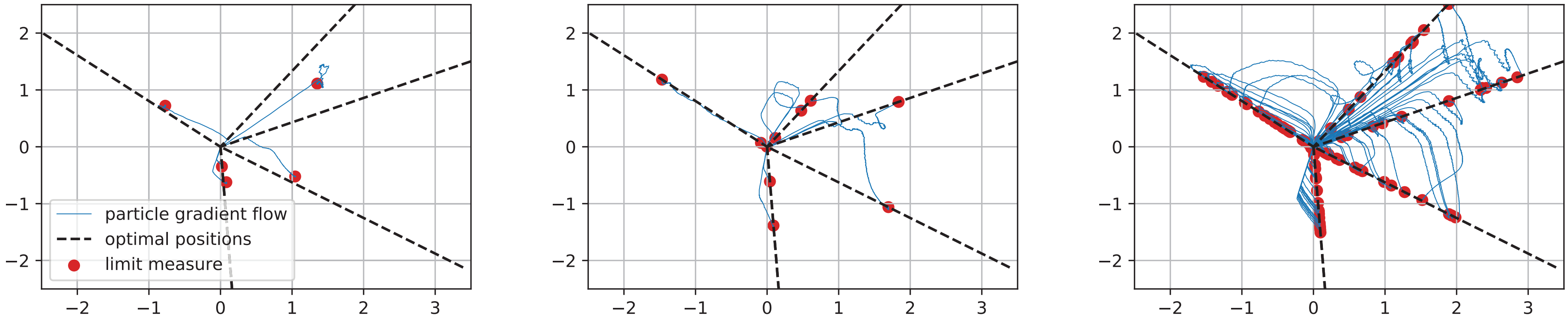

5 neurons — 10 neurons — 100 neurons

NB : also applies to spike deconvolution

From optimization to statistics

- **Summary**: with $h(x) = \frac{1}{m}\sum_{j=1}^{m} \Psi(w_j)(x) = \frac{1}{m}\sum_{j=1}^{m} \theta_2(j)\big(\theta_1(\cdot,j)^\top x\big)_+$
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- **Multiple-pass SGD or full GD** with R the empirical risk
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  - Should overfit?

Interpolation regime

- Minimizing $R(h) = \frac{1}{n}\sum_{i=1}^{n}\ell(y_i, h(x_i))$ for $h(x) = \frac{1}{m}\sum_{j=1}^{m}\theta_2(j)\big(\theta_1(\cdot, j)^\top x\big)_+$
  - When $m(d+1) > n$, typically there exist many h such that

$$\forall i \in \{1, \dots, n\}, \quad h(x_i) = y_i \qquad \text{(or } \ell(y_i, h(x_i)) = 0\text{)}$$

  - See Belkin et al. (2018); Ma et al. (2018); Vaswani et al. (2019)

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- **Which h is the gradient flow converging to?**
  - Implicit bias of (stochastic) gradient descent
  - Typically minimum Euclidean norm solution (Gunasekar et al., 2017; Soudry et al., 2018; Gunasekar et al., 2018)
  - Surprisingly difficult for the square loss
  - Surprisingly easy for the logistic loss

Maximum margin and logistic regression

- **Logistic regression:** $\displaystyle \min_{\theta \in \mathbb{R}^d} \quad \frac{1}{n} \sum_{i=1}^{n} \log(1 + \exp(-y_i \theta^\top x_i))$
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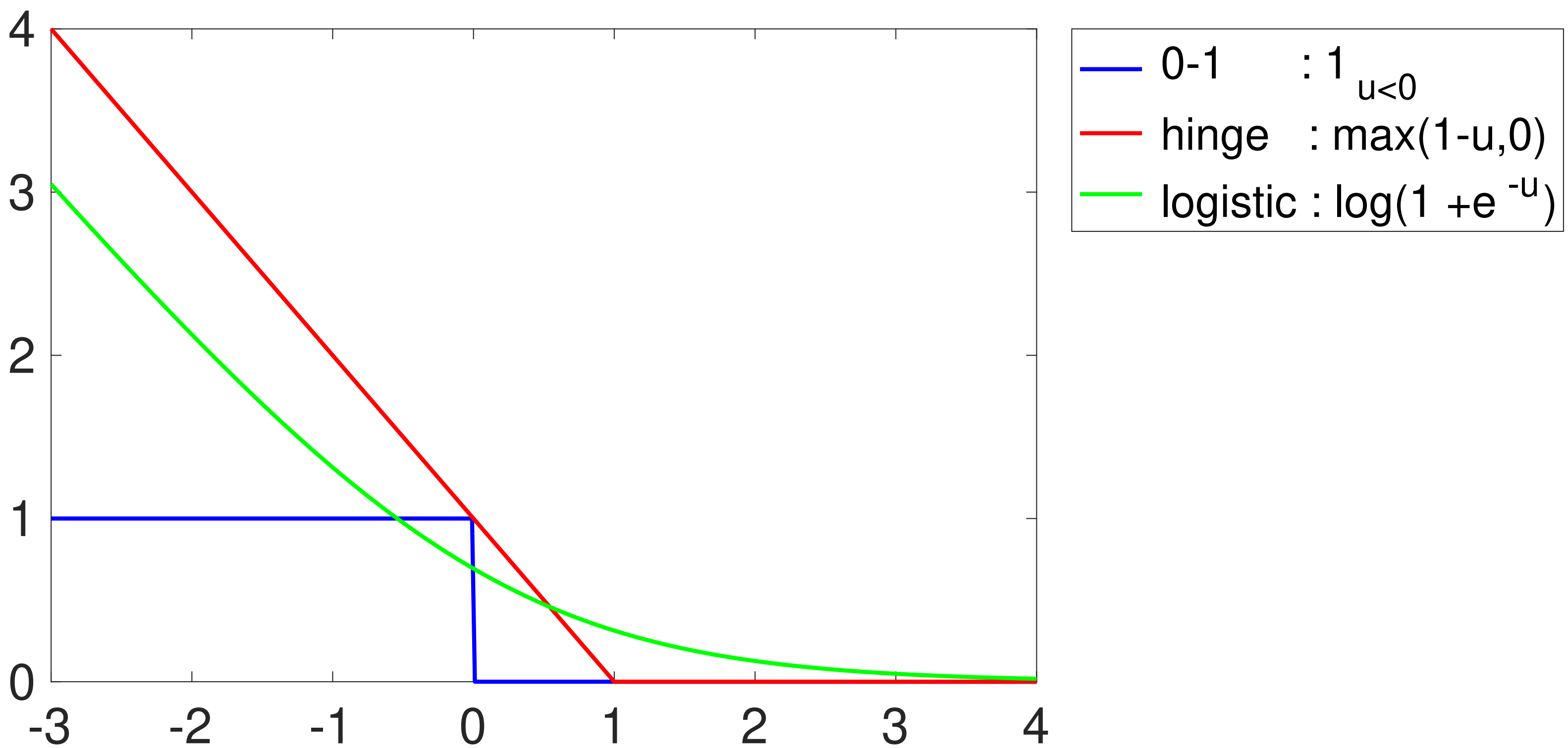

(with $u = y_i\theta^\top x_i$)

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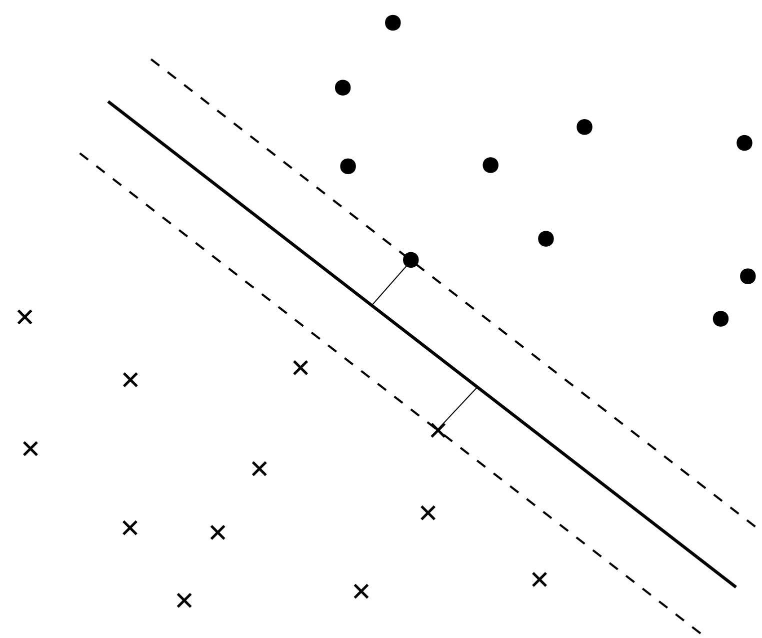
- **Implicit bias of gradient descent** (Soudry et al., 2018)
  - GD diverges but $\frac{1}{\|\theta_t\|_2}\theta_t$ converges to maximum margin separator

$$\max_{\|\eta\|_2=1} \quad \min_{i\in\{1,\dots,n\}} \ y_i\eta^\top x_i$$

  - often written as

$$\min \|\theta\|_2^2 \text{ such that } \forall i, y_i\theta^\top x_i > 1$$

  - Separable support vector machine (Vapnik and Chervonenkis, 1964)



Logistic regression for two-layer neural networks

$$h(x) = \frac{1}{m} \sum_{j=1}^{m} \theta_2(j) \big(\theta_1(\cdot, j)^\top x \big)_+$$

- **Overparameterized regime** $m \to +\infty$
  - Will converge to well-defined "maximum margin" separator

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- **Two different regimes** (Chizat and Bach, 2020)
  1. Optimizing over output layer only θ_2: random feature kernel
  2. Optimizing over all layers θ_1, θ_2: feature learning

Random feature kernel regime - I

- **Prediction function** $h(x) = \dfrac{1}{m}\sum_{j=1}^{m}\theta_2(j)\big(\theta_1(\cdot,j)^\top x\big)_+$
  - Input weights $\theta_1(\cdot,j)$, $j=1,\dots,m$, random and fixed
  - Optimize over output weights $\theta_2 \in \mathbb{R}^m$
  - Corresponds to linear predictor with $\Phi(x)_j = \frac{1}{\sqrt{m}}\big(\theta_1(\cdot,j)^\top x\big)_+$

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- **Converges to separator with minimum norm** $\|\theta_2\|_2^2$
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  - Limit when m tends to infinity?

- **Kernel** $\Phi(x)^\top \Phi(x') = \frac{1}{m}\sum_{j=1}^{m} \big(\theta_1(\cdot,j)^\top x\big)_+ \big(\theta_1(\cdot,j)^\top x'\big)_+$
  - Converges to $\mathbb{E}_\eta (\eta^\top x)_+ (\eta^\top x')_+$
  - "Random features" (Neal, 1995; Rahimi and Recht, 2007)

Random feature kernel regime - II

- **Limiting kernel** $\mathbb{E}_\eta (\eta^\top x)_+ (\eta^\top x')_+$
  - Reproducing kernel Hilbert spaces (RKHS) (see, e.g., Schölkopf and Smola, 2001)
  - Space of (very) smooth functions (Bach, 2017)

Random feature kernel regime - II

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  - Space of (very) smooth functions (Bach, 2017)

- **(informal) theorem** (Chizat and Bach, 2020): when $m \to +\infty$, the gradient flow converges to the function in the RKHS that separates the data with minimum RKHS norm
  - Quantitative analysis available
  - Letting $m \to +\infty$ is useless in practice
  - See Montanari et al. (2019) for related work in the context of "double descent"

From RKHS norm to variation norm

- **Alternative definition of the RKHS norm**

$$\|f\|^2 = \inf_{a(\cdot)} \int_{\mathbb{S}^d} |a(\eta)|^2 d\tau(\eta) \ \text{ such that } \ f(x) = \int_{\mathbb{S}^d} (\eta^\top x)_+ a(\eta) d\tau(\eta)$$

  - Input weigths uniformly distributed on the sphere (Bach, 2017)
  - Smooth functions (does not allow single hidden neuron)

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- **Variation norm** (Kurkova and Sanguineti, 2001)

$$\Omega(f) = \inf_{a(\cdot)} \int_{\mathbb{S}^d} |a(\eta)| d\tau(\eta) \;\; \text{such that} \;\; f(x) = \int_{\mathbb{S}^d} (\eta^\top x)_+ a(\eta) d\tau(\eta)$$

  – Larger space including non-smooth functions
  – Allows single hidden neuron
  – Adaptivity to linear structures (Bach, 2017)

Feature learning regime

- **Prediction function** $h(x) = \dfrac{1}{m}\sum_{j=1}^{m} \theta_2(j)\big(\theta_1(\cdot,j)^\top x\big)_+$
  - Optimize over all weights θ_1, θ_2

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  - Optimize over all weights θ_1, θ_2
- **(informal) theorem** (Chizat and Bach, 2020): when $m \to +\infty$, the gradient flow converges to the function that separates the data with minimum **variation norm**
  - Actual learning of representations
  - Adaptivity to linear structures (see Chizat and Bach, 2020)
  - No known convex optimization algorithms in polynomial time
  - End of the curve of double descent (Belkin et al., 2018)

Optimizing over two layers

- Two-dimensional classification with “bias” term

Space of parameters

- Plot of $|\theta_2(j)|\theta_1(\cdot, j)$
- Color depends on sign of $\theta_2(j)$
- “tanh” radial scale

Space of predictors

- $(+/-)$ training set
- One color per class
- Line shows 0 level set of h

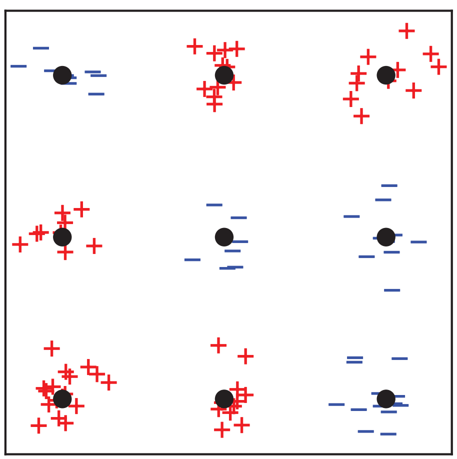
Comparison of kernel and feature learning regimes

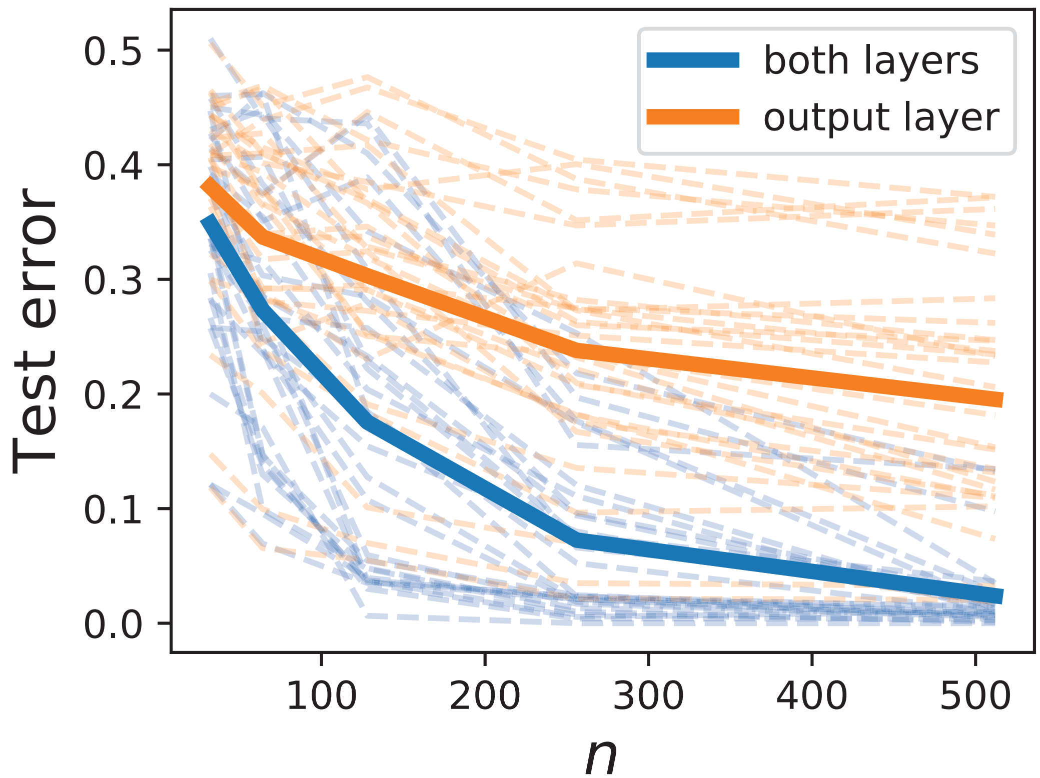
- ℓ_2 (left: kernel) vs. ℓ_1 (right: feature learning and variation norm)

Comparison of kernel and feature learning regimes

- **Adaptivity to linear structures**

- **Two-class classification in dimension** $d = 15$
  - Two first coordinates as shown below
  - All other coordinates uniformly at random





Conclusion

- **Summary**
  - Qualitative analysis of gradient descent for 2-layer neural networks
  - Global convergence with infinitely many neurons
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- **Open problems**
  - Quantitative analysis in terms of number of neurons m and time t
  - Extension to convolutional neural networks
  - Extension to deep neural networks
  - Relationships between theory and practice

Can learning theory resist deep learning?

- **Empirical successes of deep learning cannot be ignored**
  - Understanding core principles and influencing practitioners

- **Scientific standards should not be lowered**
  - Critics and limits of theoretical and empirical results
  - Rigor beyond mathematical guarantees

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- **Some wisdom from physics:**

  Physical Review adheres to the following policy with respect to use of terms such as "new" or "novel:" All material accepted for publication in the Physical Review is expected to contain new results in physics. Phrases such as "new," "for the first time," etc., therefore should normally be unnecessary; they are not in keeping with the journal's scientific style. Furthermore, such phrases could be construed as claims of priority, which the editors cannot assess and hence must rule out.

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