Fundamentals of Machine Learning for Distributed Systems

Francis Bach

INRIA - Ecole Normale Supérieure, Paris, France

Summer school on distributed learning, Sept. 2023

Slides available at www.di.ens.fr/~fbach/rsd2023.pdf

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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**

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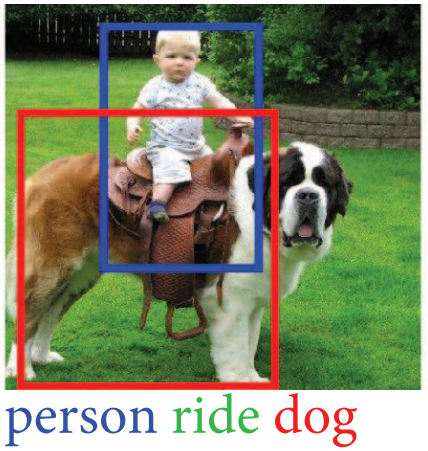
  - Scientific: from bioinformatics to humanities
- **Need for automated processing of massive data**
- **Series of "hypes"**

  Big data $\rightarrow$ Data science $\rightarrow$ Machine Learning
  $\rightarrow$ Deep Learning $\rightarrow$ Artificial Intelligence

Recent progress in perception (vision, audio, text)

From translate.google.fr



From Peyré et al. (2017)

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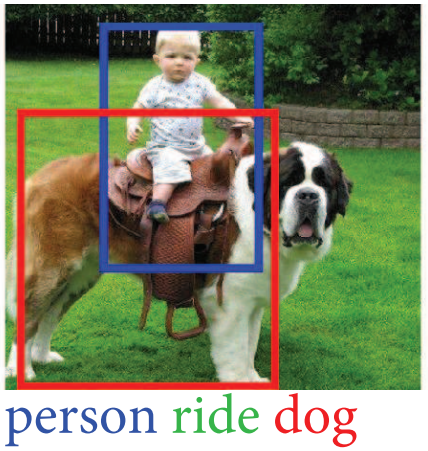

From Peyré et al. (2017)

(1) **Massive data**

(2) **Computing power**

(3) **Methodological and scientific progress**

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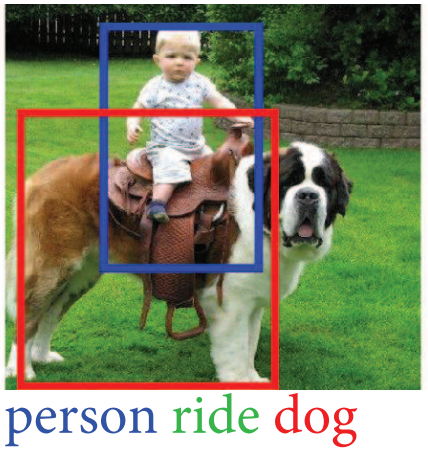

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"Intelligence" = models + algorithms + data
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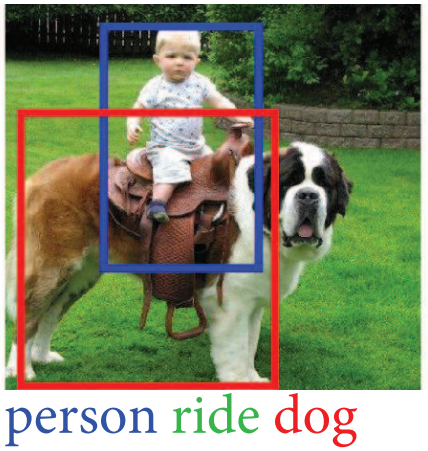

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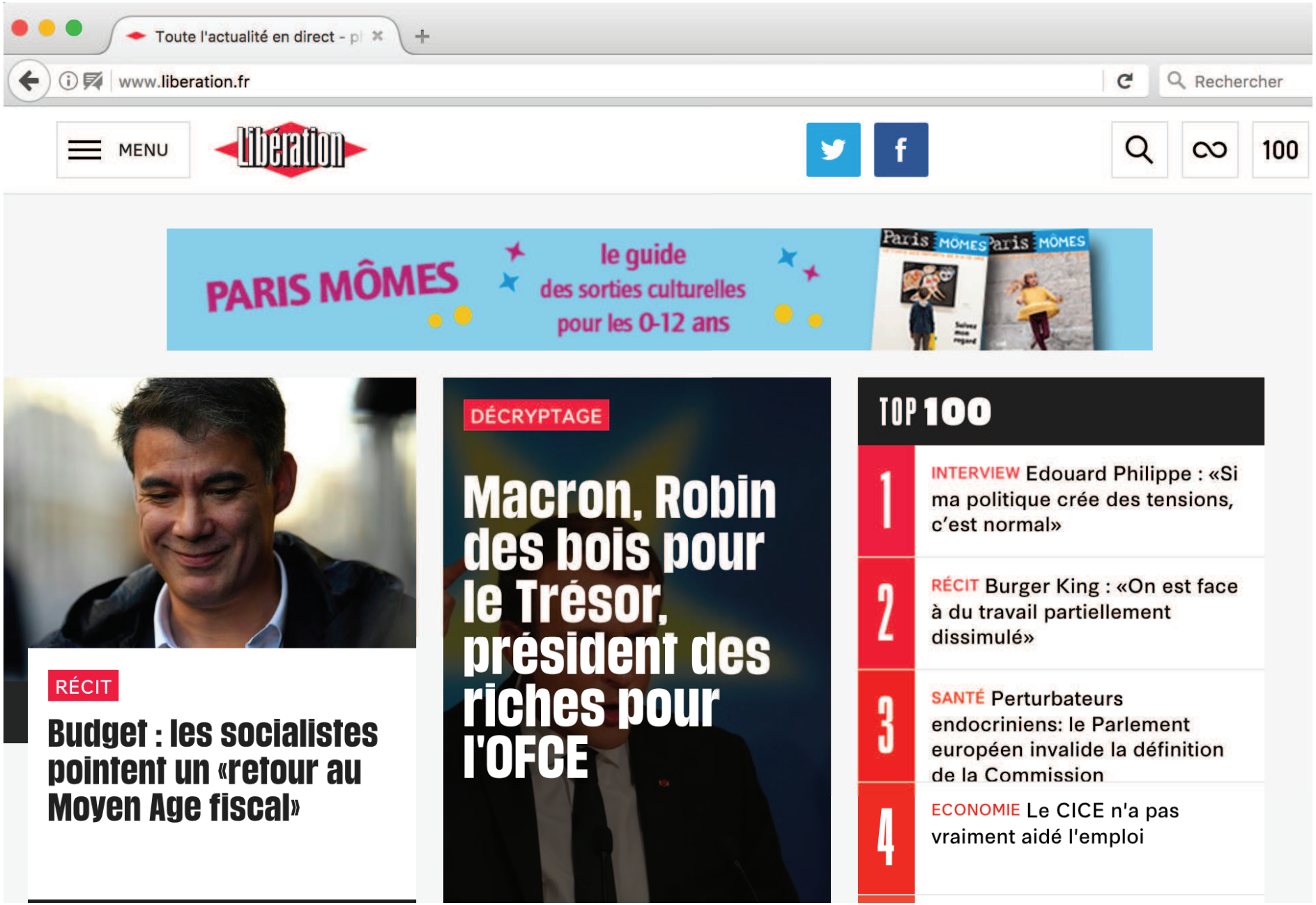
Machine learning for large-scale data

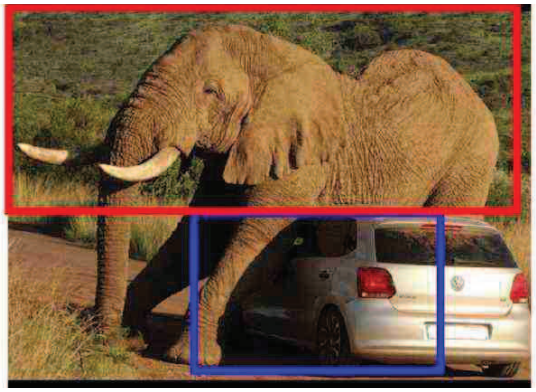
- **Large-scale supervised machine learning**: **large d, large n**
  - d : dimension of each observation (input) or number of parameters
  - n : number of observations

- **Examples**: computer vision, advertising, bioinformatics, etc.

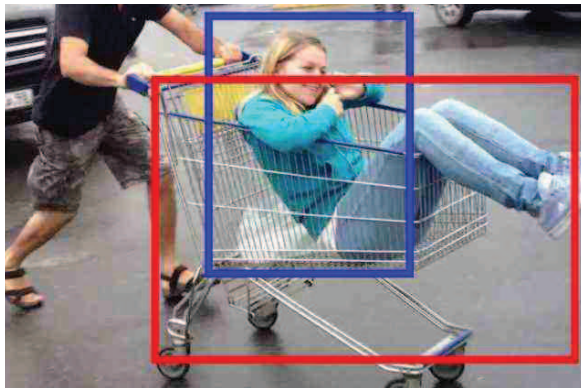
Advertising



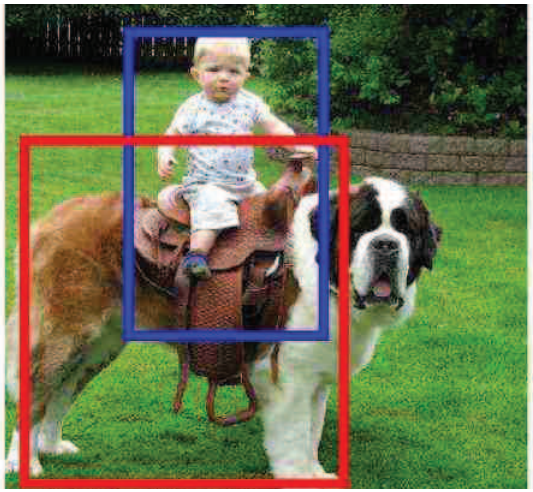
Object / action recognition in images



car under elephant



person in cart

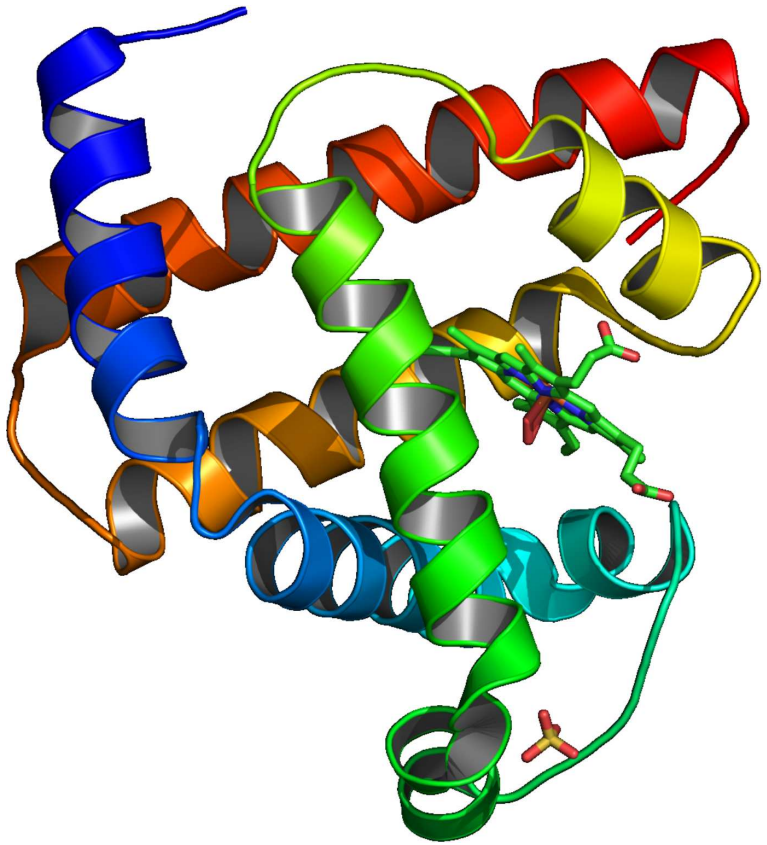


person ride dog

person on top of traffic light

From Peyré, Laptev, Schmid and Sivic (2017)

Bioinformatics



- Predicting multiple functions and interactions of **proteins**
- **Massive data**: up to 1 millions for humans!
- **Complex data**
  - Amino-acid sequence
  - Link with DNA
  - Tri-dimensional molecule

Machine learning for large-scale data

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  - Stochastic gradient methods (Robbins and Monro, 1951)
- **Goal: Present classical algorithms and some recent progress**

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- **Goal: Present classical algorithms and some recent progress**
  - *Disclaimer: Significant focus on optimization*

Outline

1. **Introduction/motivation: Supervised machine learning**
   - Machine learning $\approx$ optimization of finite sums
   - Batch optimization methods

2. **Fast stochastic gradient methods for convex problems**
   - Variance reduction: for *training* error
   - Single pass SGD: for *testing* error

3. **Beyond convex problems**
   - Generic algorithms with generic "guarantees"
   - Global convergence for over-parameterized neural networks

Parametric supervised machine learning

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

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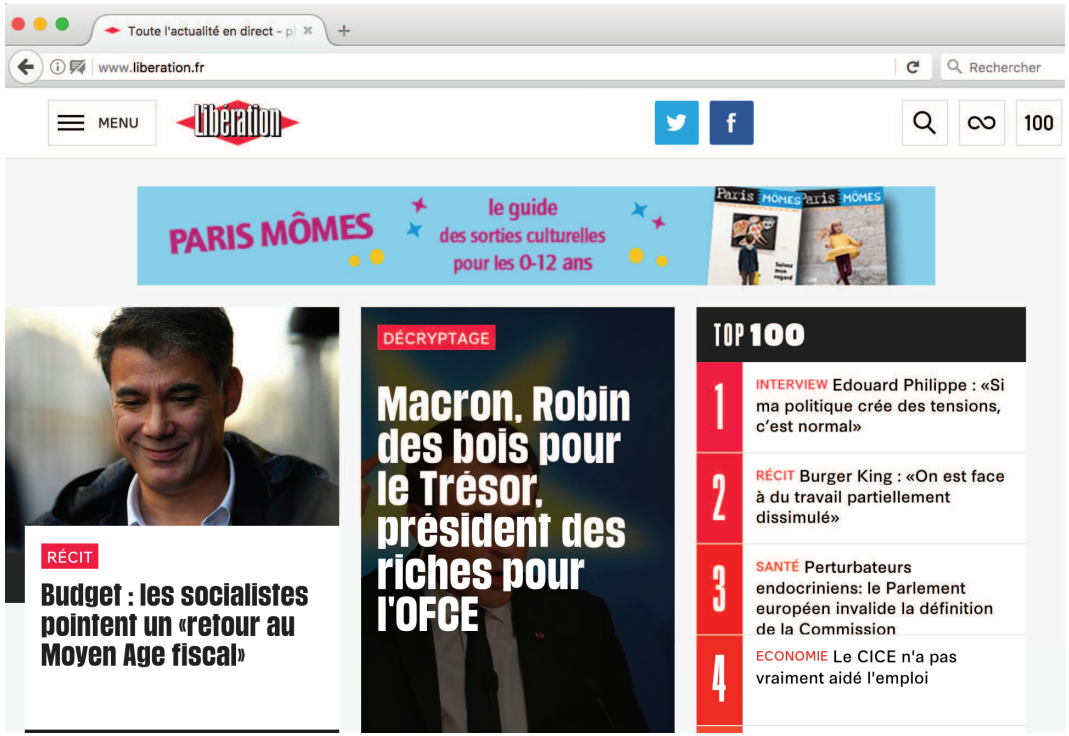

- **Advertising**: $n > 10^9$
  - $\Phi(x) \in \{0, 1\}^d$, $d > 10^9$
  - Navigation history + ad

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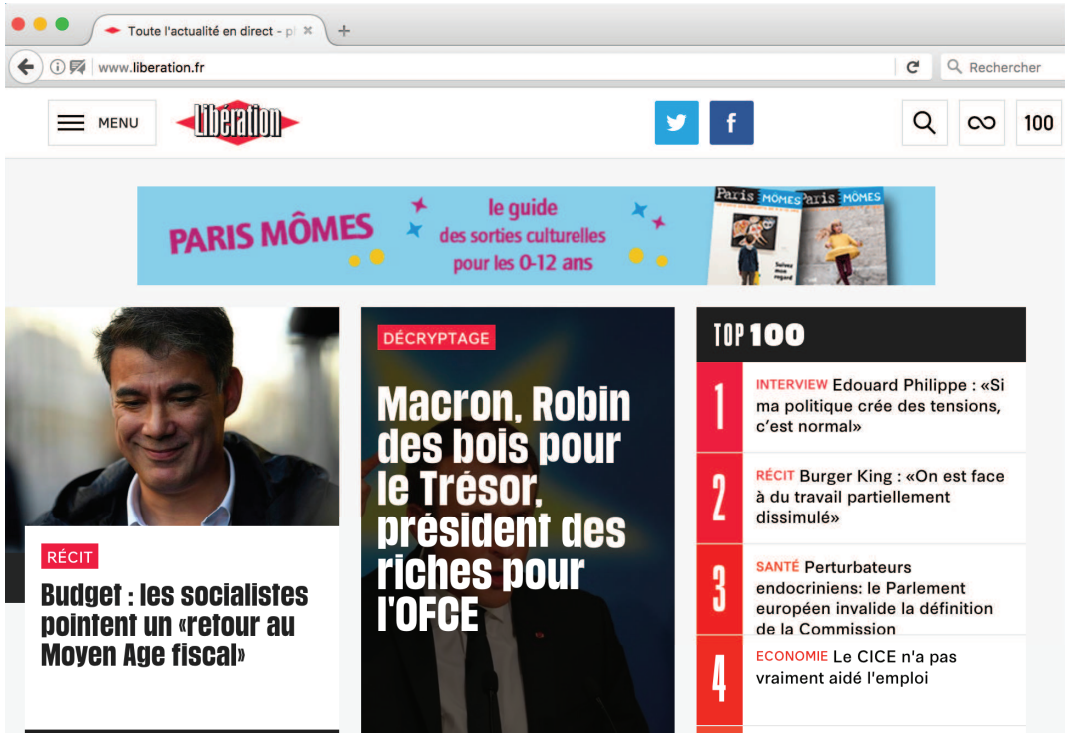

- **Advertising**: $n > 10^9$
  - $\Phi(x) \in \{0, 1\}^d$, $d > 10^9$
  - Navigation history + ad
- Linear predictions
  - $h(x, \theta) = \theta^\top \Phi(x)$

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x_1 x_2 x_3 x_4 x_5 x_6

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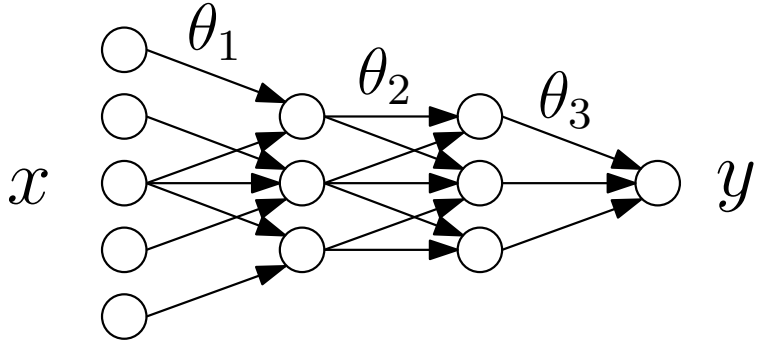
- Neural networks $(n, d > 10^6)$: $h(x, \theta) = \theta_m^\top \sigma(\theta_{m-1}^\top \sigma(\cdots \theta_2^\top \sigma(\theta_1^\top x))$



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- **(regularized) empirical risk minimization**: find $\hat{\theta}$ solution of

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

data fitting term + regularizer

Usual losses

- **Regression**: $y \in \mathbb{R}$, prediction $\hat{y} = h(x, \theta)$
  - quadratic loss $\frac{1}{2}(y - \hat{y})^2 = \frac{1}{2}(y - h(x, \theta))^2$

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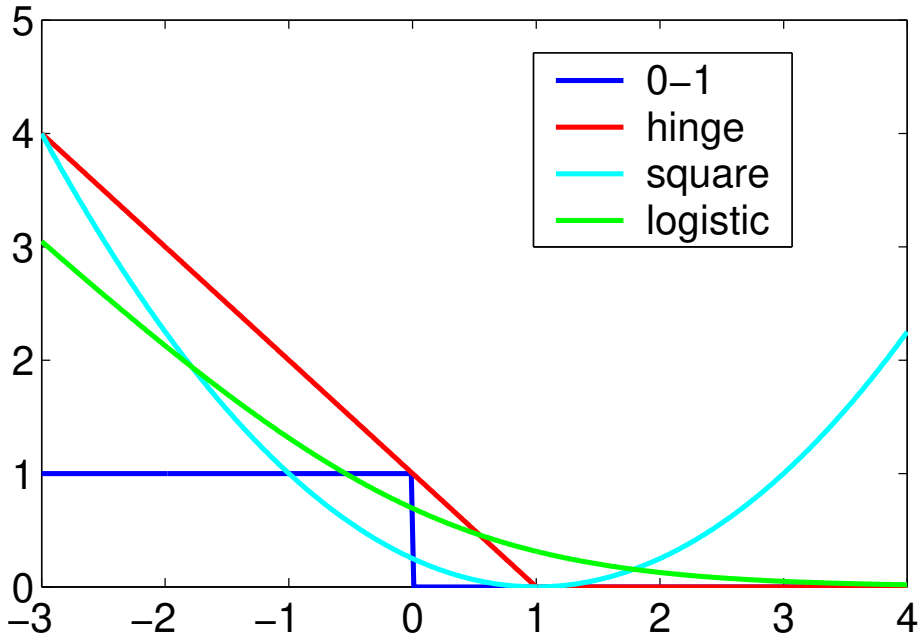
- **Classification** : $y \in \{-1, 1\}$, prediction $\hat{y} = \text{sign}(h(x, \theta))$
  - loss of the form $\ell(y\, h(x, \theta))$
  - "True" 0-1 loss: $\ell(y\, h(x, \theta)) = 1_{y\, h(x,\theta)<0}$
  - Usual convex losses:



Usual regularizers

- **Main goal**: avoid overfitting
- **(squared) Euclidean norm**: $\|\theta\|_2^2 = \sum_{j=1}^{d} |\theta_j|^2$
  - Numerically well-behaved if $h(x, \theta) = \theta^\top \Phi(x)$
  - Representer theorem and kernel methods : $\theta = \sum_{i=1}^{n} \alpha_i \Phi(x_i)$
  - See, e.g., Schölkopf and Smola (2001); Shawe-Taylor and Cristianini (2004)

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- **Sparsity-inducing norms**
  - Main example: ℓ_1-norm $\|\theta\|_1 = \sum_{j=1}^d |\theta_j|$
  - Perform model selection as well as regularization
  - Non-smooth optimization and structured sparsity
  - See, e.g., Bach, Jenatton, Mairal, and Obozinski (2012a,b)

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data fitting term + regularizer

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- Optimization: optimization of regularized risk training cost

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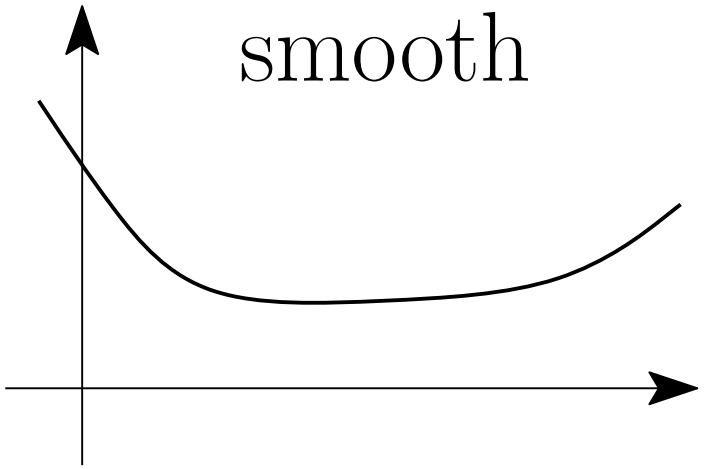
data fitting term + regularizer

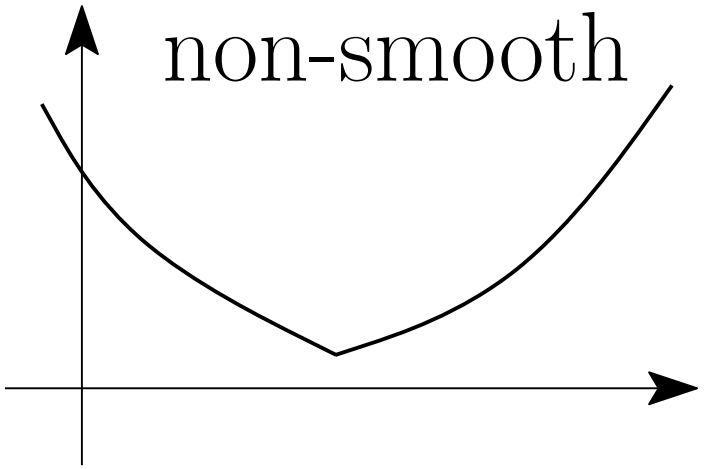
- Optimization: optimization of regularized risk — training cost
- Statistics: guarantees on $\mathbb{E}_{p(x,y)} \ell(y, h(x, \theta))$ — testing cost

Smoothness and (strong) convexity

- A function $g : \mathbb{R}^d \to \mathbb{R}$ is L-smooth if and only if it is twice differentiable and

$$\forall \theta \in \mathbb{R}^d, \ \left|\text{eigenvalues}\left[g''(\theta)\right]\right| \leqslant L$$





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- **Machine learning**
  - with $g(\theta) = \frac{1}{n} \sum_{i=1}^n \ell(y_i, h(x_i, \theta))$
  - Smooth prediction function $\theta \mapsto h(x_i, \theta)$ + smooth loss
  - *(see next slide)*

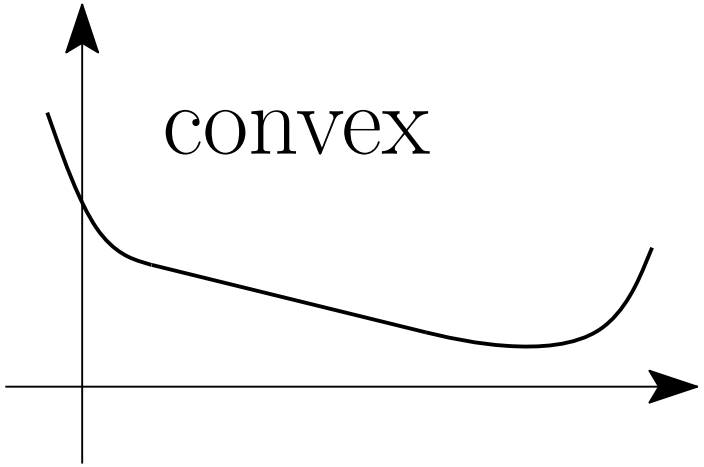
Board

- Function $g(\theta) = \frac{1}{n} \sum_{i=1}^n \ell(y_i, \theta^\top \Phi(x_i))$
- Gradient $g'(\theta) = \frac{1}{n} \sum_{i=1}^n \ell'(y_i, \theta^\top \Phi(x_i)) \Phi(x_i)$
- Hessian $g''(\theta) = \frac{1}{n} \sum_{i=1}^n \ell''(y_i, \theta^\top \Phi(x_i)) \Phi(x_i) \Phi(x_i)^\top$
  - Smooth loss $\Rightarrow \ell''(y_i, \theta^\top \Phi(x_i))$ bounded

Smoothness and (strong) convexity

- A twice differentiable function $g : \mathbb{R}^d \to \mathbb{R}$ is convex if and only if

$$\forall \theta \in \mathbb{R}^d, \text{ eigenvalues}\big[g''(\theta)\big] \geqslant 0$$



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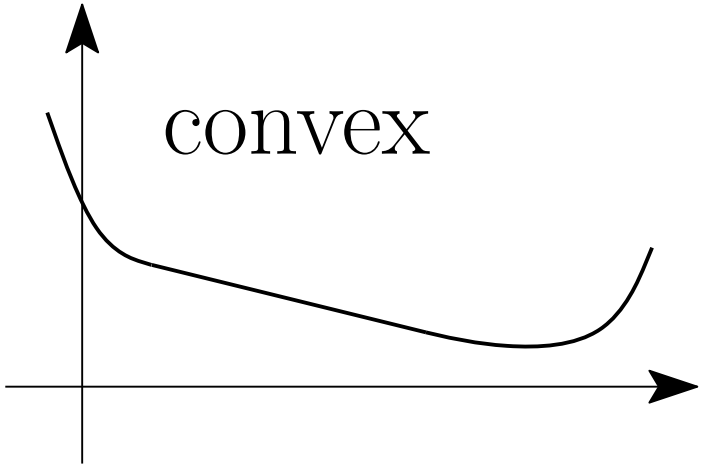

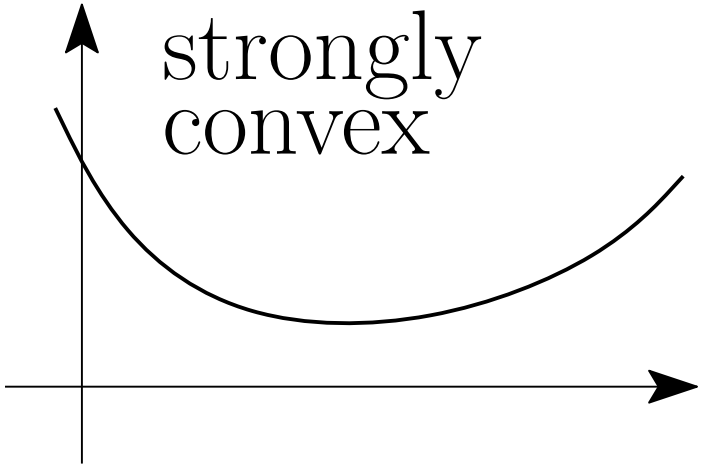

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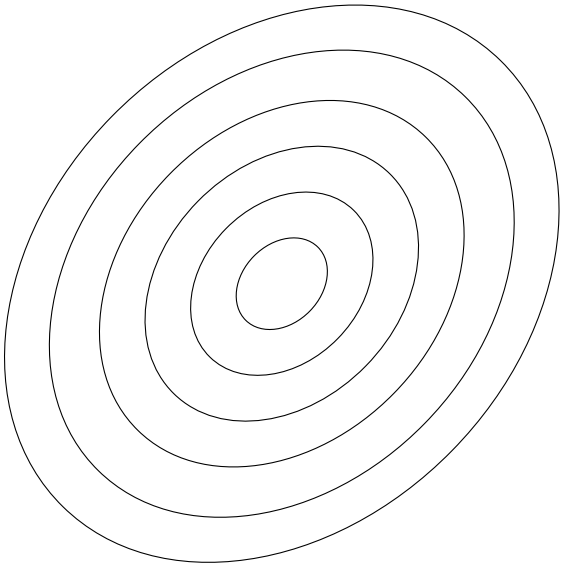
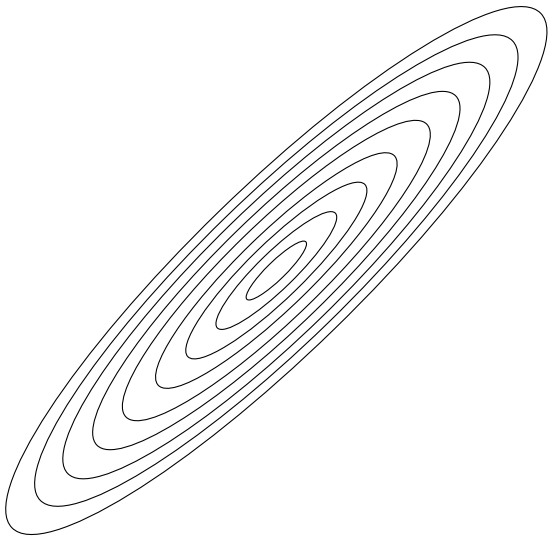
  - Condition number $\kappa = L/\mu \geqslant 1$



(small $\kappa = L/\mu$)



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- **Convexity in machine learning**
  - With $g(\theta) = \frac{1}{n} \sum_{i=1}^n \ell(y_i, h(x_i, \theta))$
  - Convex loss and linear predictions $h(x, \theta) = \theta^\top \Phi(x)$

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- **Relevance of convex optimization**
  - Easier design and analysis of algorithms
  - Global minimum vs. local minimum vs. stationary points
  - Gradient-based algorithms only need convexity for their analysis

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- **Strong convexity in machine learning**
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  - Invertible covariance matrix $\frac{1}{n}\sum_{i=1}^n \Phi(x_i)\Phi(x_i)^\top \Rightarrow n \geqslant d$ *(slide)*
  - Even when $\mu > 0$, μ may be arbitrarily small!

Board

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- Gradient $g'(\theta) = \frac{1}{n} \sum_{i=1}^n \ell'(y_i, \theta^\top \Phi(x_i)) \Phi(x_i)$
- Hessian $g''(\theta) = \frac{1}{n} \sum_{i=1}^n \ell''(y_i, \theta^\top \Phi(x_i)) \Phi(x_i) \Phi(x_i)^\top$
  - Smooth loss $\Rightarrow \ell''(y_i, \theta^\top \Phi(x_i))$ bounded
- Square loss $\Rightarrow \ell''(y_i, \theta^\top \Phi(x_i)) = 1$
  - Hessian proportional to $\frac{1}{n} \sum_{i=1}^n \Phi(x_i) \Phi(x_i)^\top$

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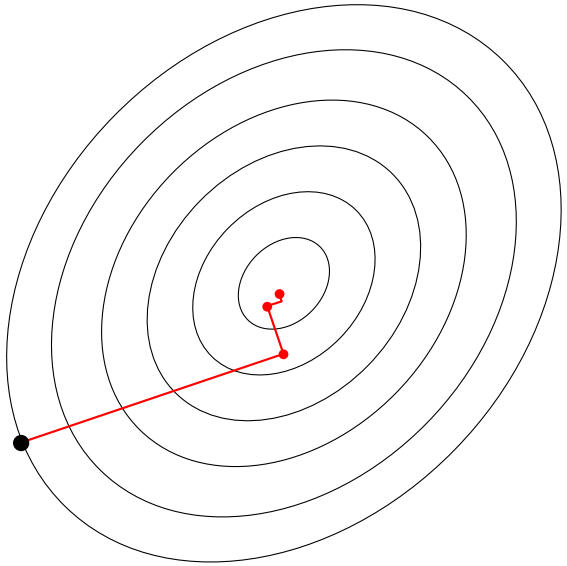
  - Invertible covariance matrix $\frac{1}{n}\sum_{i=1}^n \Phi(x_i)\Phi(x_i)^\top \Rightarrow n \geqslant d$ *(slide)*
  - Even when $\mu > 0$, μ may be arbitrarily small!

- **Adding regularization by $\frac{\mu}{2}\|\theta\|^2$**
  - creates additional bias unless μ is small, but reduces variance
  - Typically $\sqrt{n} \leqslant \kappa = L/\mu \leqslant n$

Iterative methods for minimizing smooth functions

- **Assumption**: g convex and L-smooth on $\mathbb{R}^d$
- **Gradient descent**: $\theta_t = \theta_{t-1} - \gamma_t \, g'(\theta_{t-1})$ *(line search)*



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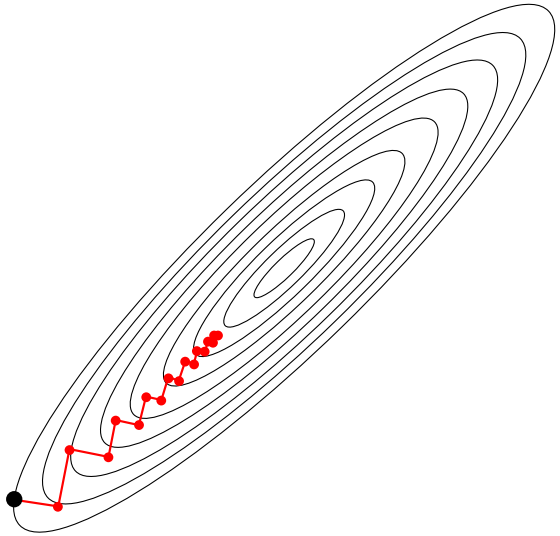

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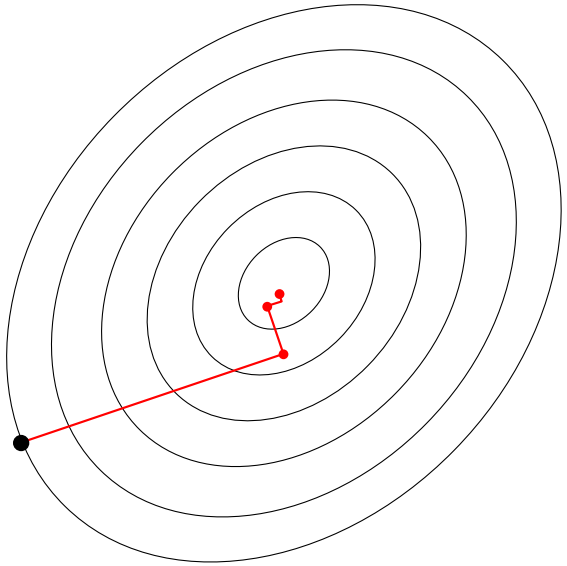
$$g(\theta_t) - g(\theta_*) \leqslant O(1/t)$$
$$g(\theta_t) - g(\theta_*) \leqslant O((1-\mu/L)^t) = O(e^{-t(\mu/L)}) \text{ if } \mu\text{-strongly convex}$$



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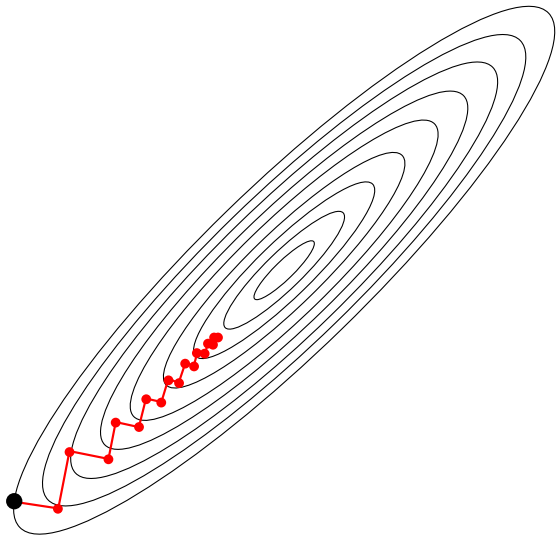

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- **Newton method**: $\theta_t = \theta_{t-1} - g''(\theta_{t-1})^{-1} g'(\theta_{t-1})$
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   - Generic algorithms with generic "guarantees"
   - Global convergence for over-parameterized neural networks

Parametric supervised machine learning

- **Data**: n observations $(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}$, $i = 1, \dots, n$, **i.i.d.**
- **Prediction function** $h(x, \theta) \in \mathbb{R}$ parameterized by $\theta \in \mathbb{R}^d$
- **(regularized) empirical risk minimization**: find $\hat{\theta}$ solution of

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

data fitting term + regularizer

- Optimization: optimization of regularized risk — training cost
- Statistics: guarantees on $\mathbb{E}_{p(x,y)} \ell(y, h(x, \theta))$ — testing cost

Stochastic gradient descent (SGD) for finite sums

$$\min_{\theta \in \mathbb{R}^d} g(\theta) = \frac{1}{n} \sum_{i=1}^{n} f_i(\theta)$$

- **Iteration**: $\theta_t = \theta_{t-1} - \gamma_t f'_{i(t)}(\theta_{t-1})$
  - Sampling with replacement: $i(t)$ random element of $\{1, \dots, n\}$
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- **Convergence rate** if each f_i is convex L-smooth and g μ-strongly-convex:

$$\mathbb{E} g(\bar{\theta}_t) - g(\theta_*) \leqslant \begin{cases} O(1/\sqrt{t}) & \text{if } \gamma_t = 1/(L\sqrt{t}) \\ O(L/(\mu t)) = O(\kappa/t) & \text{if } \gamma_t = 1/(\mu t) \end{cases}$$

  - No adaptivity to strong-convexity in general
  - Running-time complexity: $O(d \cdot \kappa/\varepsilon)$

Deterministic and stochastic methods

- Minimize $g(\theta) = \frac{1}{n}\sum_{i=1}^{n} f_i(\theta)$ with $f_i(\theta) = \ell\big(y_i, h(x_i, \theta)\big) + \lambda\Omega(\theta)$

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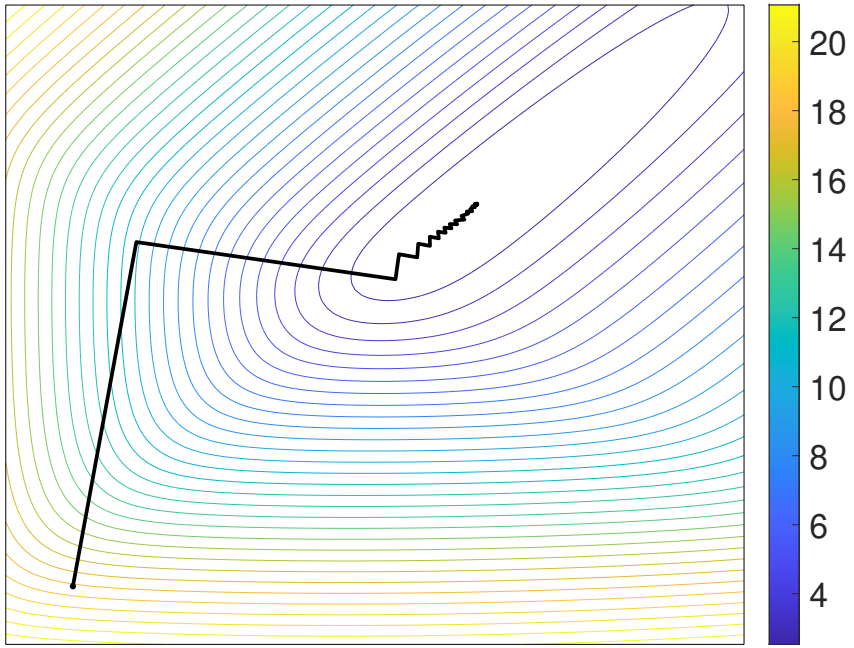
- **Gradient descent**: $\theta_t = \theta_{t-1} - \gamma\nabla g(\theta_{t-1}) = \theta_{t-1} - \frac{\gamma}{n}\sum_{i=1}^{n}\nabla f_i(\theta_{t-1})$ (Cauchy, 1847)



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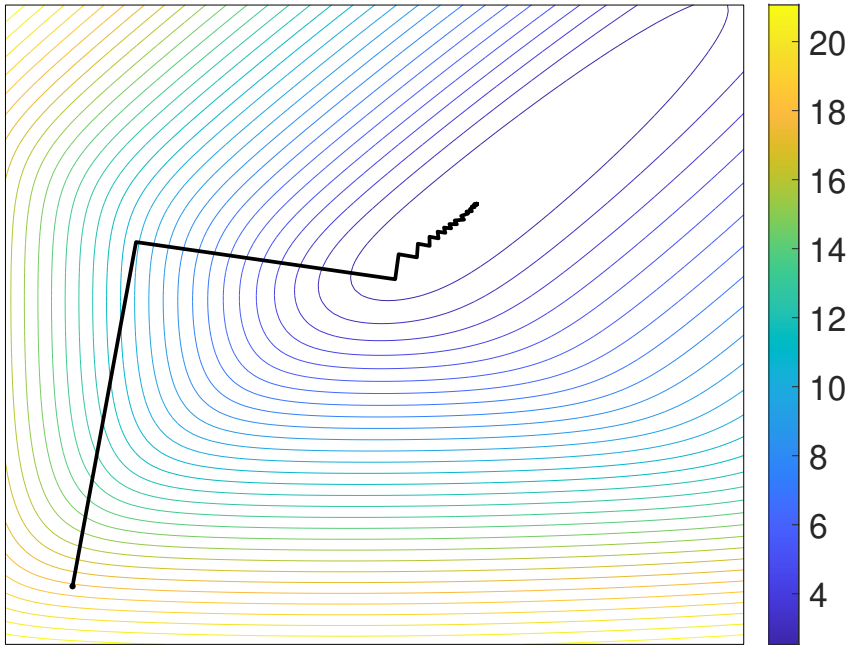
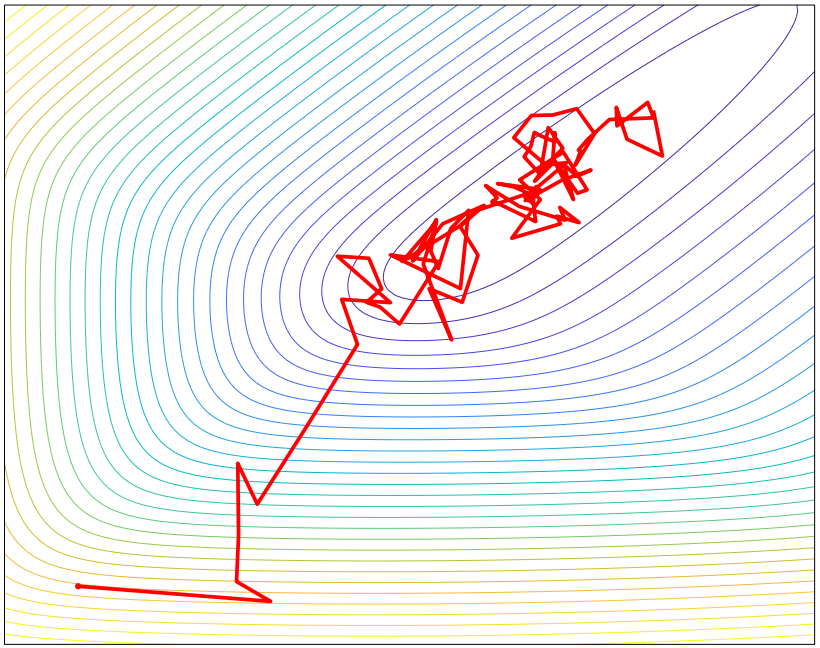
- **Stochastic gradient descent**: $\theta_t = \theta_{t-1} - \gamma\nabla f_{i(t)}(\theta_{t-1})$ (Robbins and Monro, 1951)





Stochastic gradient with exponential convergence

- **Variance reduction**
  - SAG (Le Roux, Schmidt, and Bach, 2012)
  - SVRG (Johnson and Zhang, 2013; Zhang et al., 2013)
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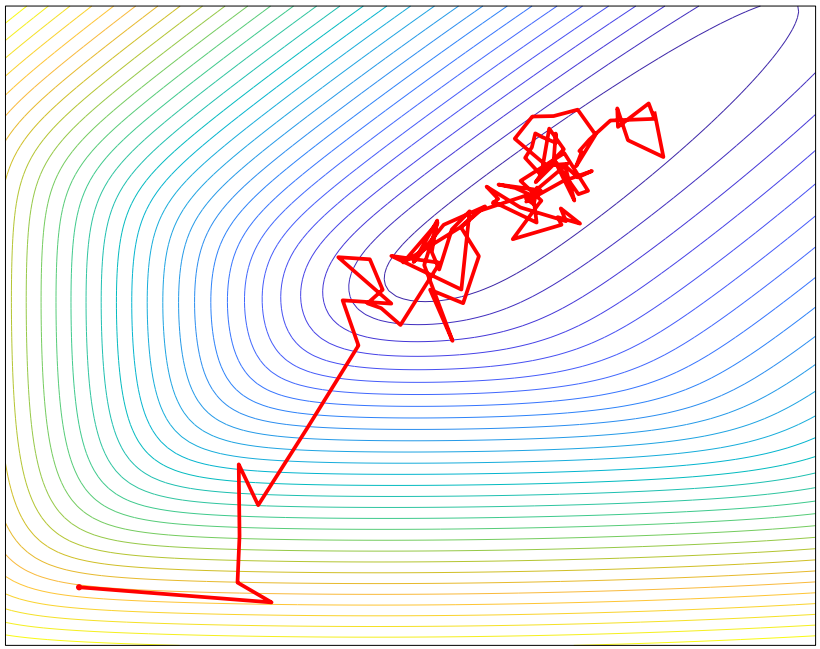
$$\theta_t = \theta_{t-1} - \gamma \left[\nabla f_{i(t)}(\theta_{t-1}) \right]$$



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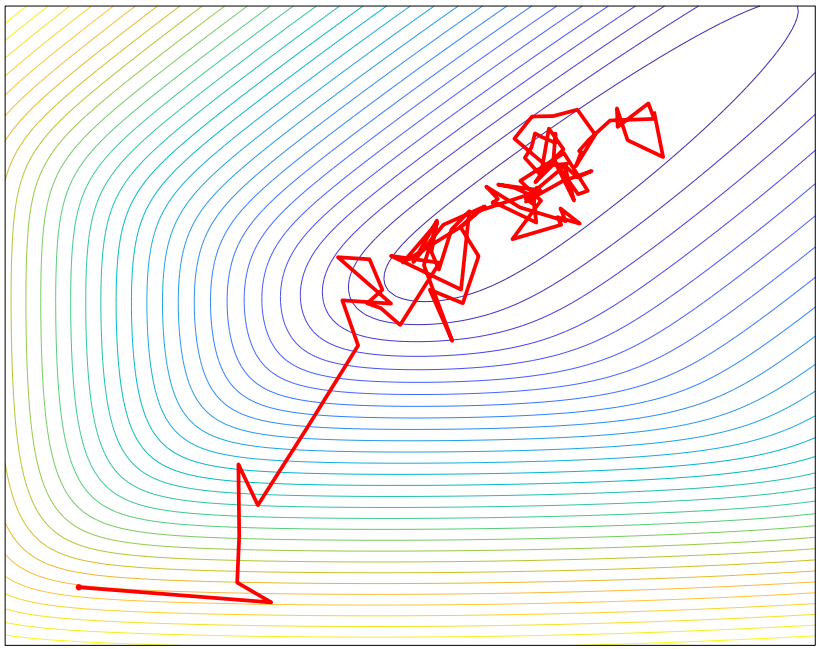

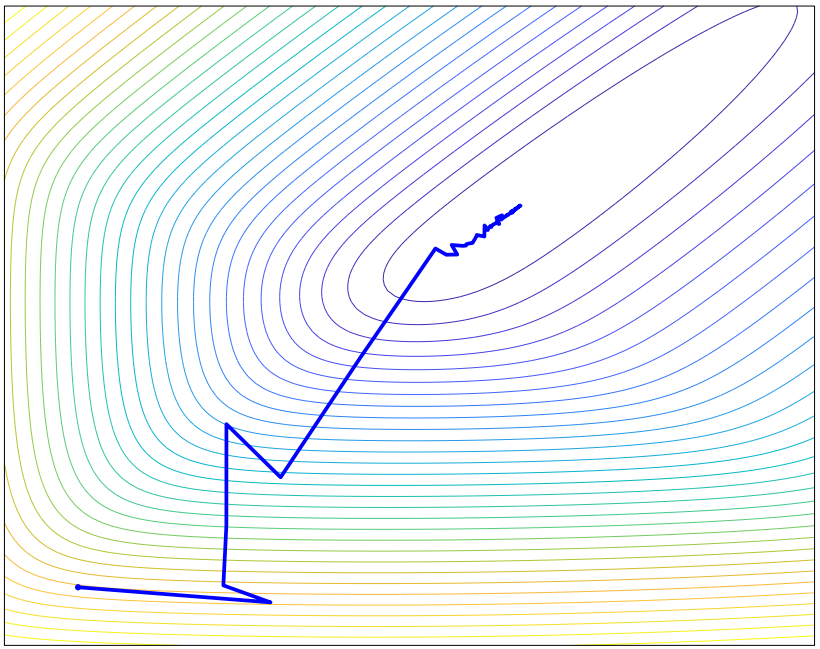

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- **Number of individual gradient computations to reach error** ε (convex objectives with condition number κ)

Gradient descent	$n\kappa \quad \times \log \frac{1}{\varepsilon}$
Stochastic gradient descent	$\kappa \quad \times \quad \frac{1}{\varepsilon}$
Variance reduction	$(n+\kappa) \quad \times \log \frac{1}{\varepsilon}$

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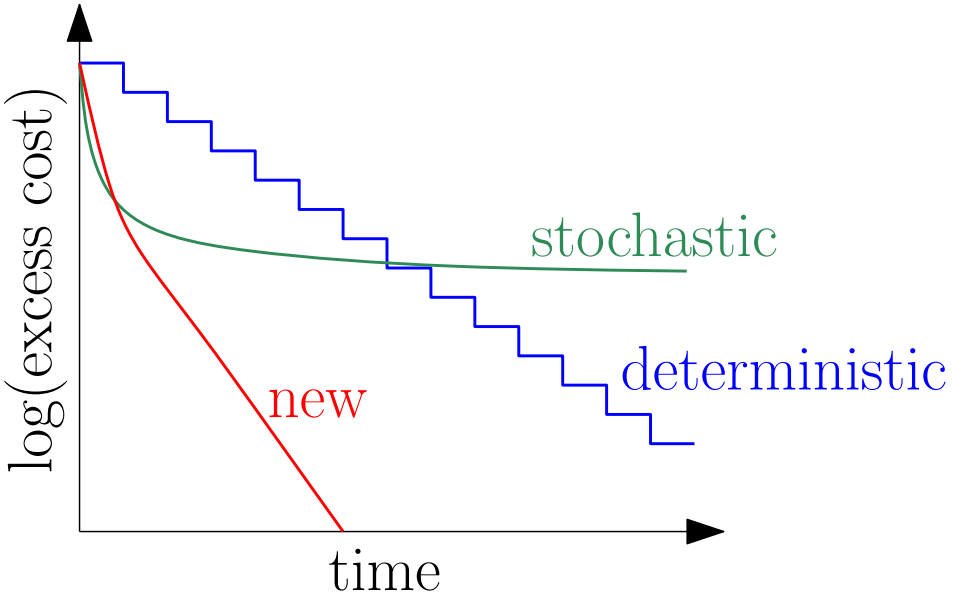
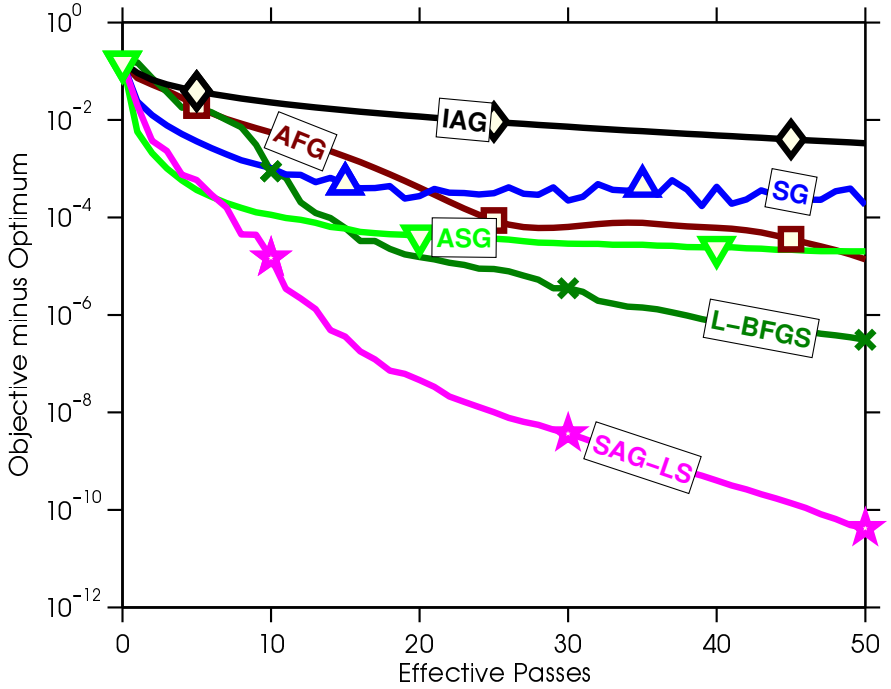
Exponentially convergent SGD for finite sums
From theory to practice and vice-versa





- **Empirical performance "matches" theoretical guarantees**

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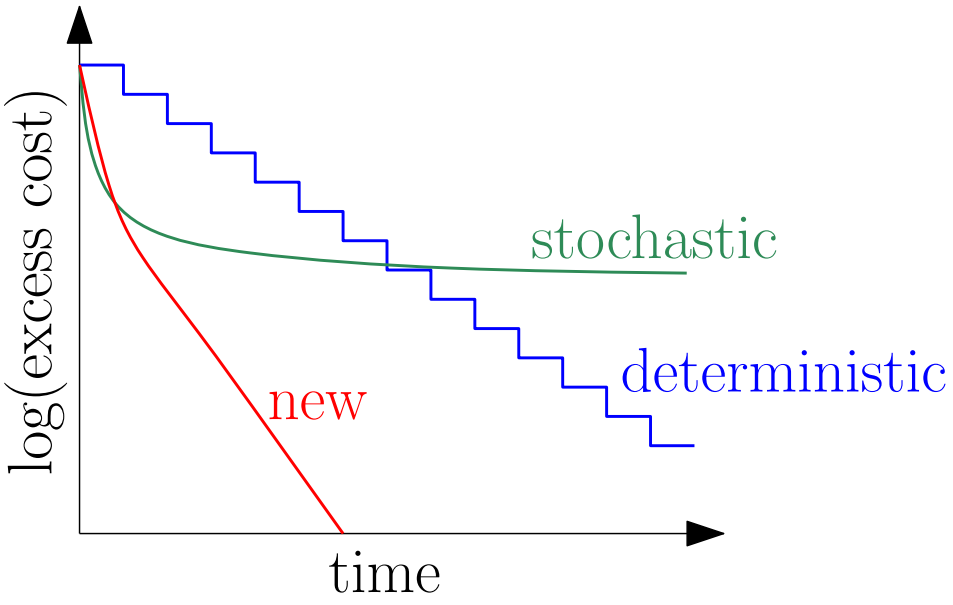
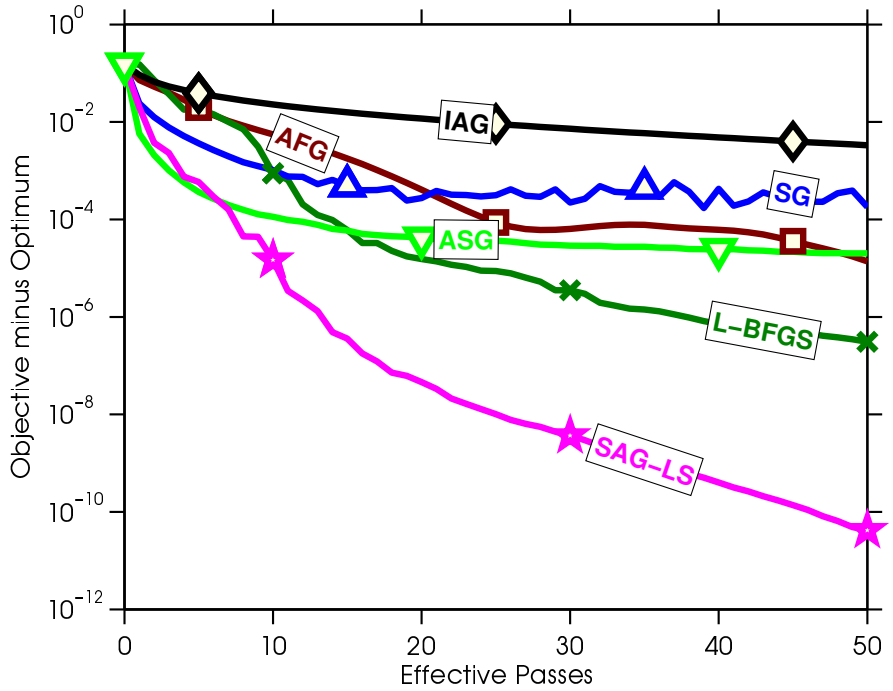
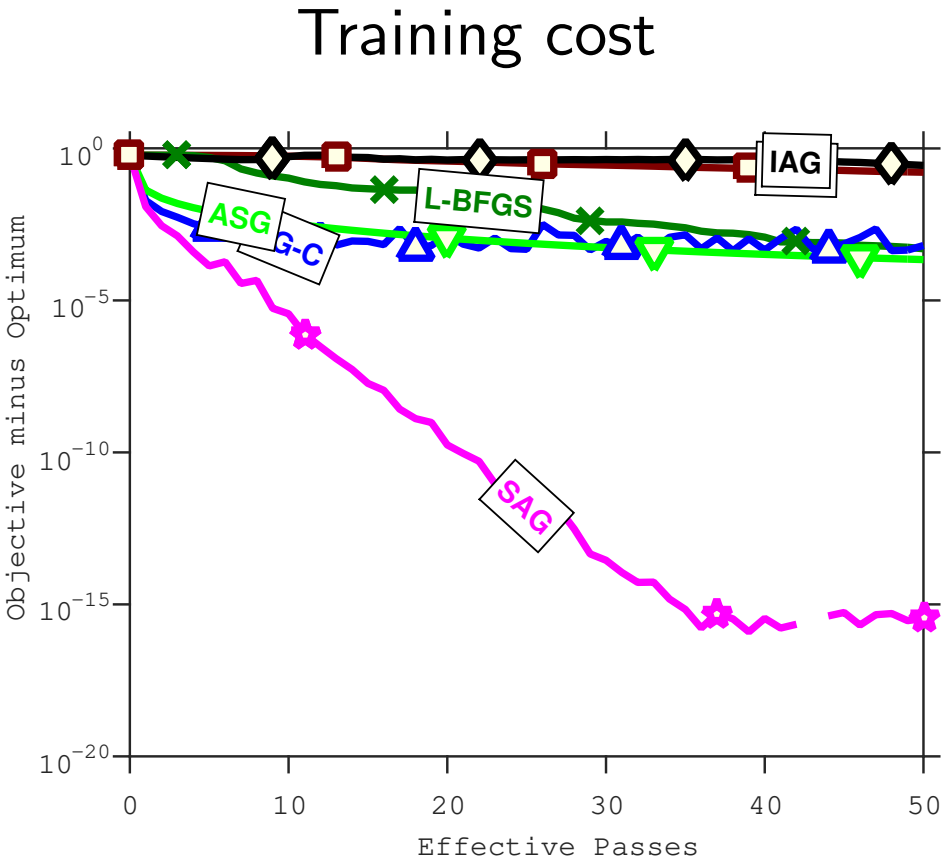




- **Empirical performance "matches" theoretical guarantees**
- **Theoretical analysis suggests practical improvements**
  - Non-uniform sampling, acceleration
  - Matching upper and lower bounds

From training to testing errors

- `rcv1` dataset ($n = 697\,641$, $d = 47\,236$)
  - NB: IAG, SG-C, ASG with optimal step-sizes in hindsight



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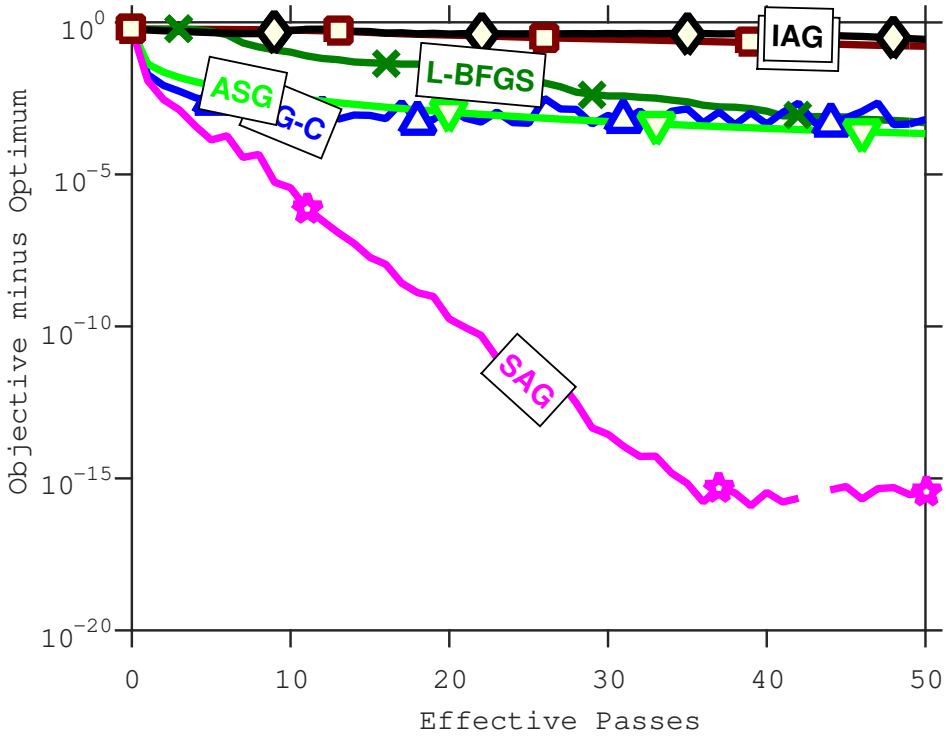
Training cost



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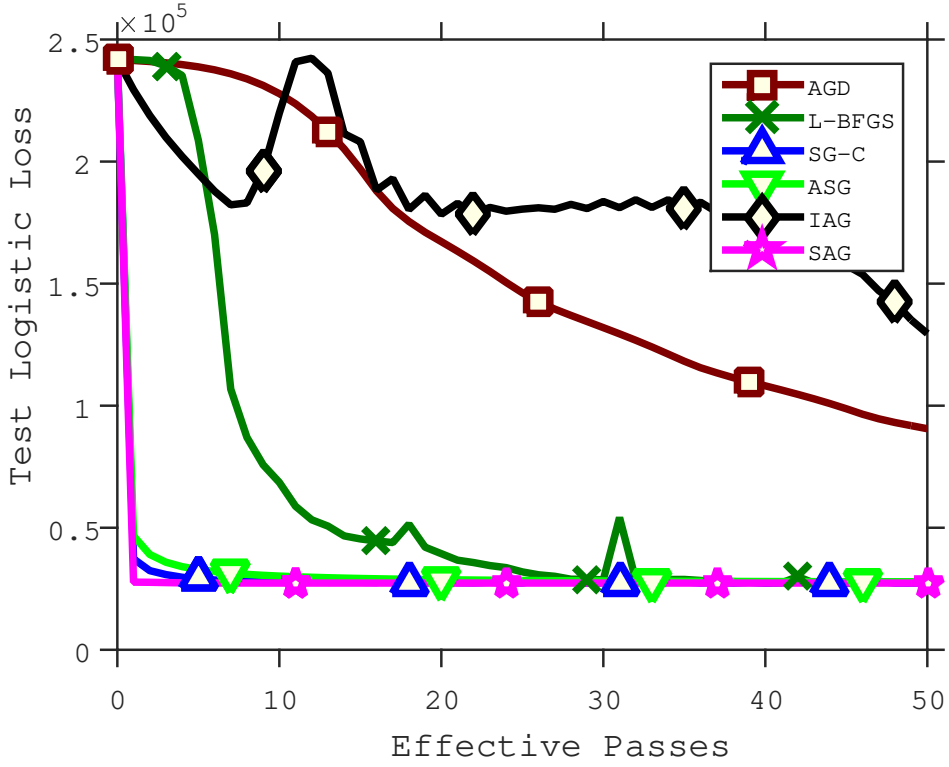

SGD minimizes the testing cost!

- **Goal**: minimize $f(\theta) = \mathbb{E}_{p(x,y)}\ell(y, h(x, \theta))$
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- **Constant-step-size SGD**
  - Convergence up to the noise level (Solodov, 1998)
  - Full convergence and robustness to ill-conditioning (Bach and Moulines, 2013)

Perspectives

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  - Provable and precise rates
  - Improves on two known lower-bounds (by using structure)
  - Several extensions / interpretations / accelerations

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  - Sampling without replacement (Gurbuzbalaban et al., 2015)
  - Parallelization (Leblond, Pedregosa, and Lacoste-Julien, 2016; Hendrikx, Bach, and Massoulié, 2019)
  - Non-convex problems (Reddi et al., 2016)

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data fitting term + regularizer

- **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 2020+)
  - Support vector machines and kernel methods
  - Inference in graphical models
  - Sparsity / low-rank models (statistics + optimization)
  - Convex relaxation of unsupervised learning problems
  - Optimal transport
  - Stochastic methods for large-scale learning and online learning

Convex optimization for machine learning
From theory to practice and vice-versa

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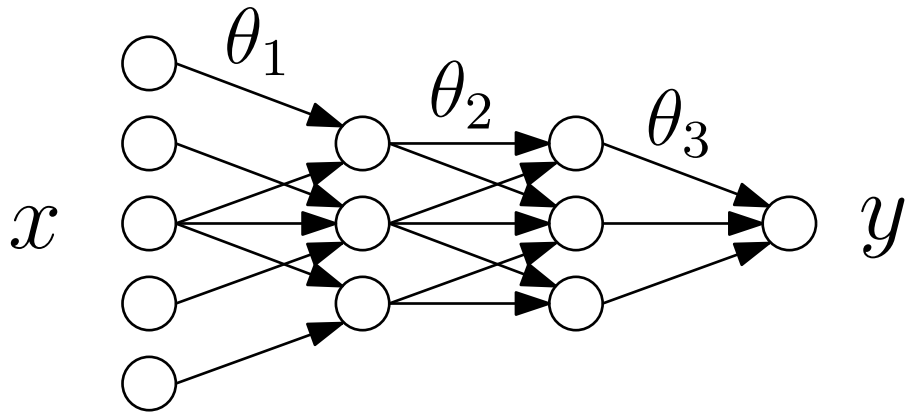
- **What about deep learning?**

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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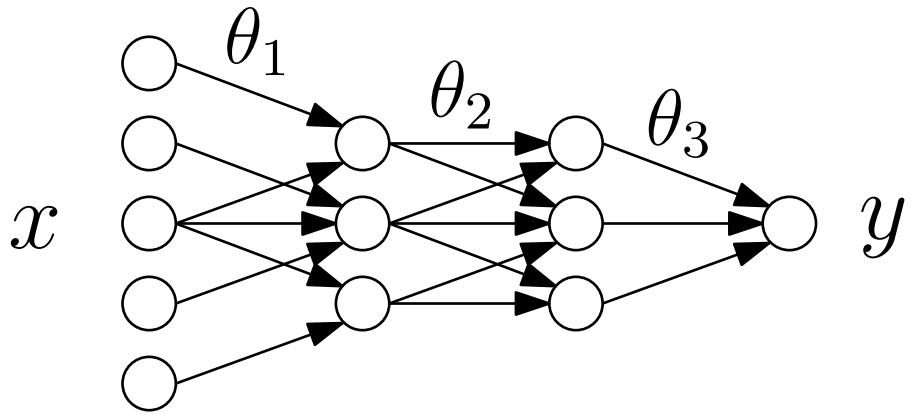

- **Generalization guarantees**
  - See "MythBusters: A Deep Learning Edition" by Sasha Rakhlin
  - Bartlett et al. (2017); Golowich et al. (2018)

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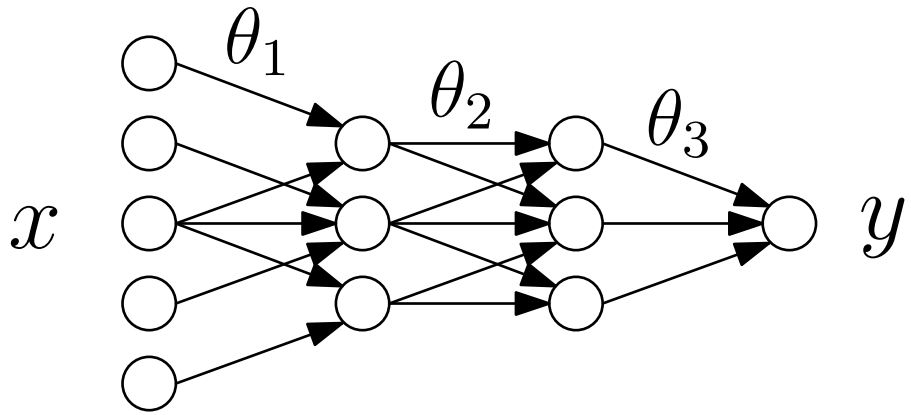
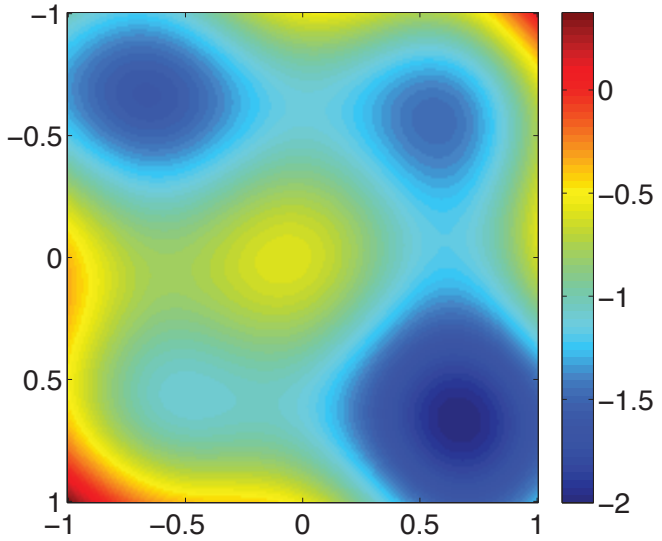


- **Generalization guarantees**
  - See "MythBusters: A Deep Learning Edition" by Sasha Rakhlin
  - Bartlett et al. (2017); Golowich et al. (2018)

- **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
  - etc...



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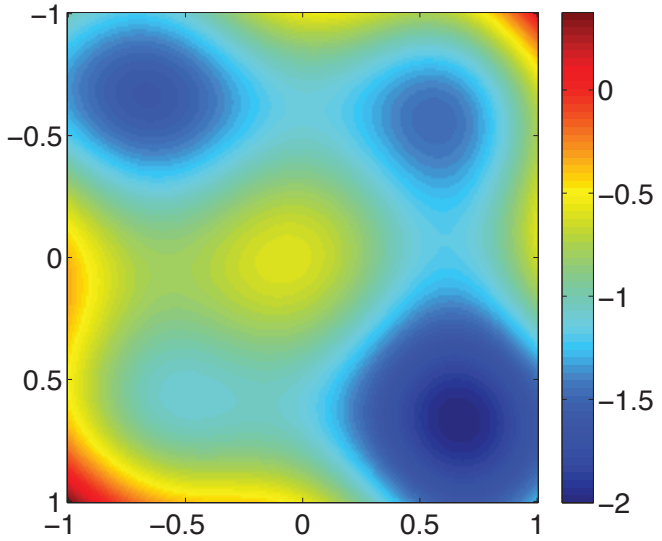

- **Generic local theoretical guarantees**
  - Convergence to stationary points or local minima
  - See, e.g., Lee et al. (2016); Jin et al. (2017)

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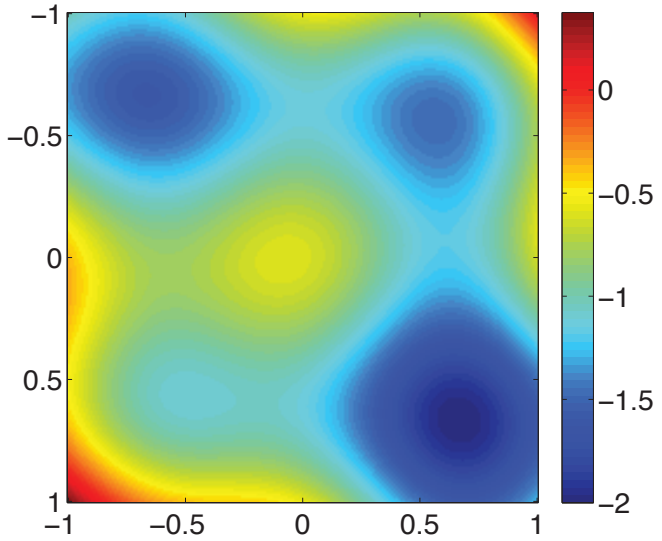
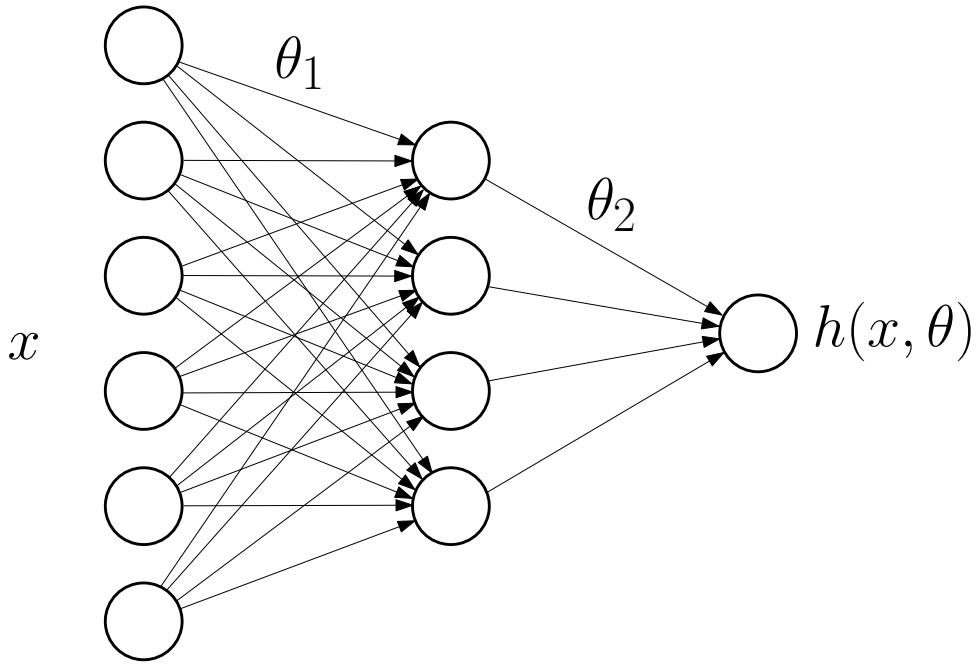


- **General global performance guarantees impossible to obtain**

Gradient descent for a single hidden layer

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

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



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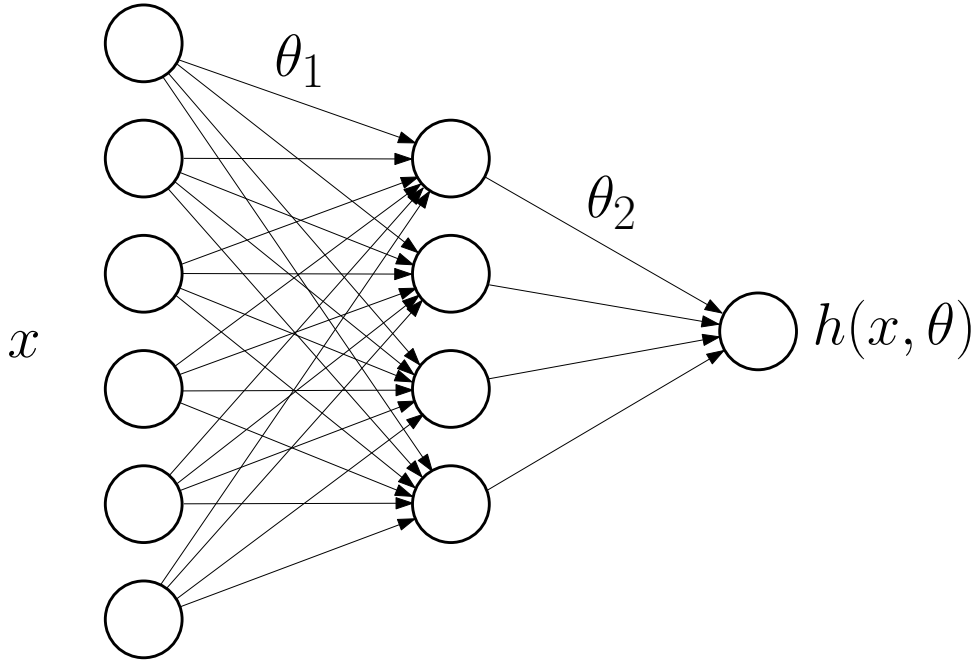

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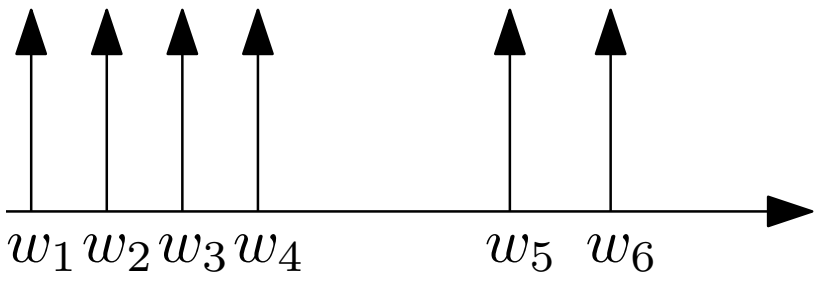

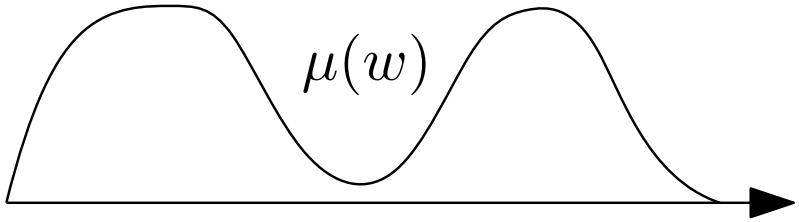

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  - Overparameterized models with m large $\approx$ measure μ with densities
  - Barron (1993); Kurkova and Sanguineti (2001); Bengio et al. (2006); Rosset et al. (2007); Bach (2017)

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
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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 $(w_1, \ldots, w_m)$

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

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 $F_m(w_1, \ldots, w_m) = R\Big(\frac{1}{m}\sum_{i=1}^{m} \Psi(w_i)\Big)$

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  - Idealization of (stochastic) gradient descent
- **Limit when m tends to infinity**
  - Wasserstein gradient flow (Nitanda and Suzuki, 2017; Chizat and Bach, 2018; Mei, Montanari, and Nguyen, 2018; Sirignano and Spiliopoulos, 2018; Rotskoff and Vanden-Eijnden, 2018)

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

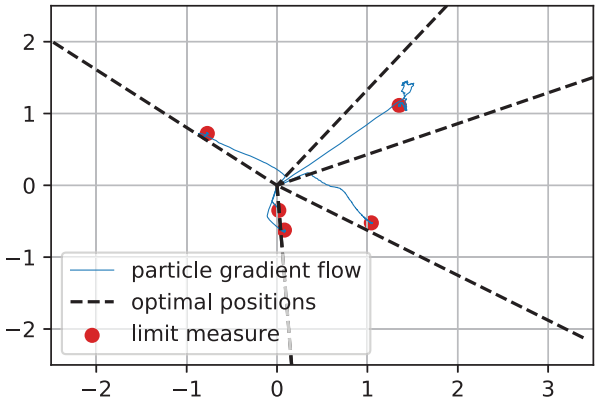
- **Two ingredients**: homogeneity and initialization

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

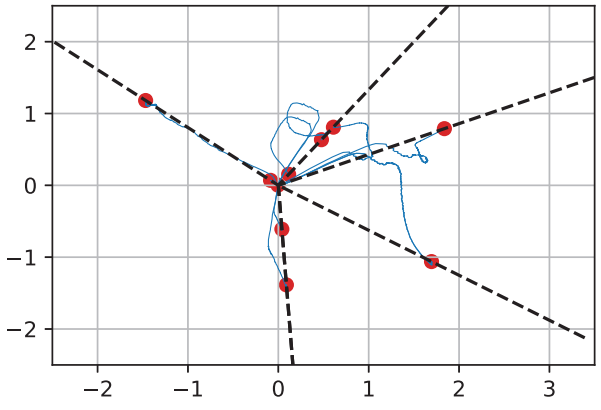
- **Two ingredients**: homogeneity and initialization
- **Homogeneity** (see, e.g., Haeffele and Vidal, 2017; Bach et al., 2008)
  - Full or partial, e.g., $\Psi(w_i)(x) = m\theta_2(i) \cdot \sigma\left[\theta_1(\cdot, i)^\top x\right]$
  - Applies to rectified linear units (but also to sigmoid activations)
- **Sufficiently spread initial measure**
  - Needs to cover the entire sphere of directions

Simple simulations with neural networks

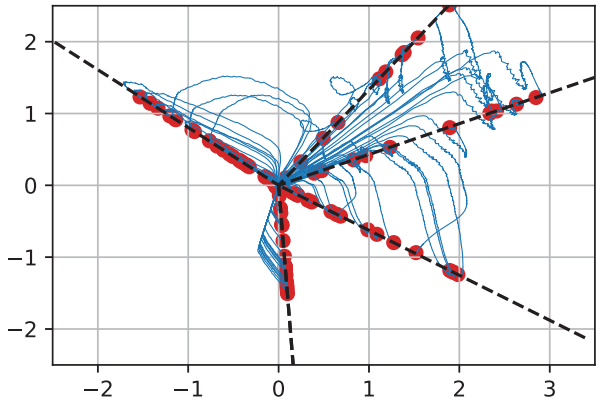
- ReLU units with $d = 2$ (optimal predictor has 5 neurons)



5 neurons



10 neurons



100 neurons

Conclusions
Optimization for machine learning

- **Well understood**
  - Convex case with a single machine
  - Matching lower and upper bounds for variants of SGD
  - Non-convex case: SGD for local risk minimization

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Optimization for machine learning

- **Well understood**
  - Convex case with a single machine
  - Matching lower and upper bounds for variants of SGD
  - Non-convex case: SGD for local risk minimization

- **Not well understood**: many open problems
  - Step-size schedules and acceleration, conditioning
  - Dealing with non-convexity
    (global minima vs. local minima and stationary points)
  - Distributed learning: multiple cores, GPUs, and cloud
  - Beyond running time

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