Optimization for Large Scale Machine Learning

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Slides available at `www.di.ens.fr/~fbach/mlss2020.pdf`

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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  Big data → Data science → Machine Learning
  → Deep Learning → Artificial Intelligence

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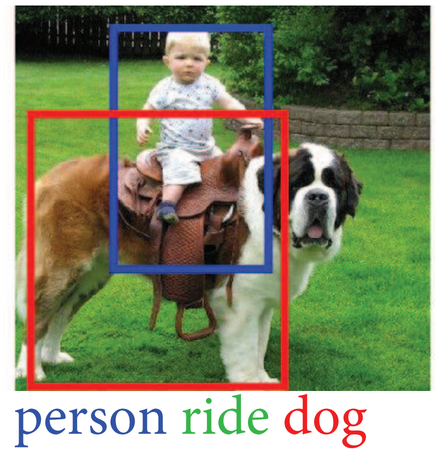
- **Series of "hypes"**

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

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

Recent progress in perception (vision, audio, text)

From translate.google.fr



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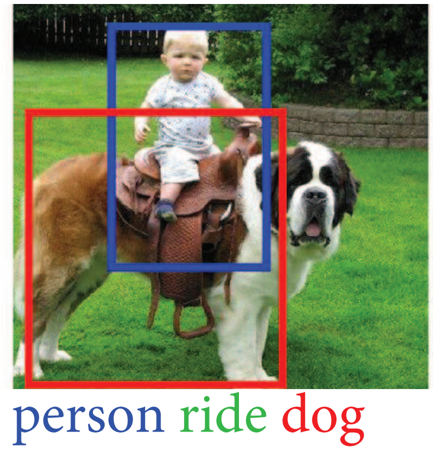

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(2) **Computing power**

(3) **Methodological and scientific progress**

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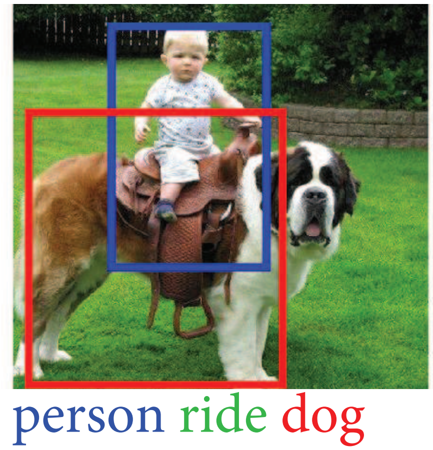

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"Intelligence" = models + algorithms + data + computing power

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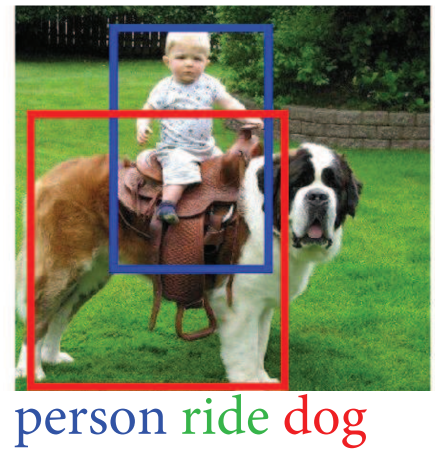

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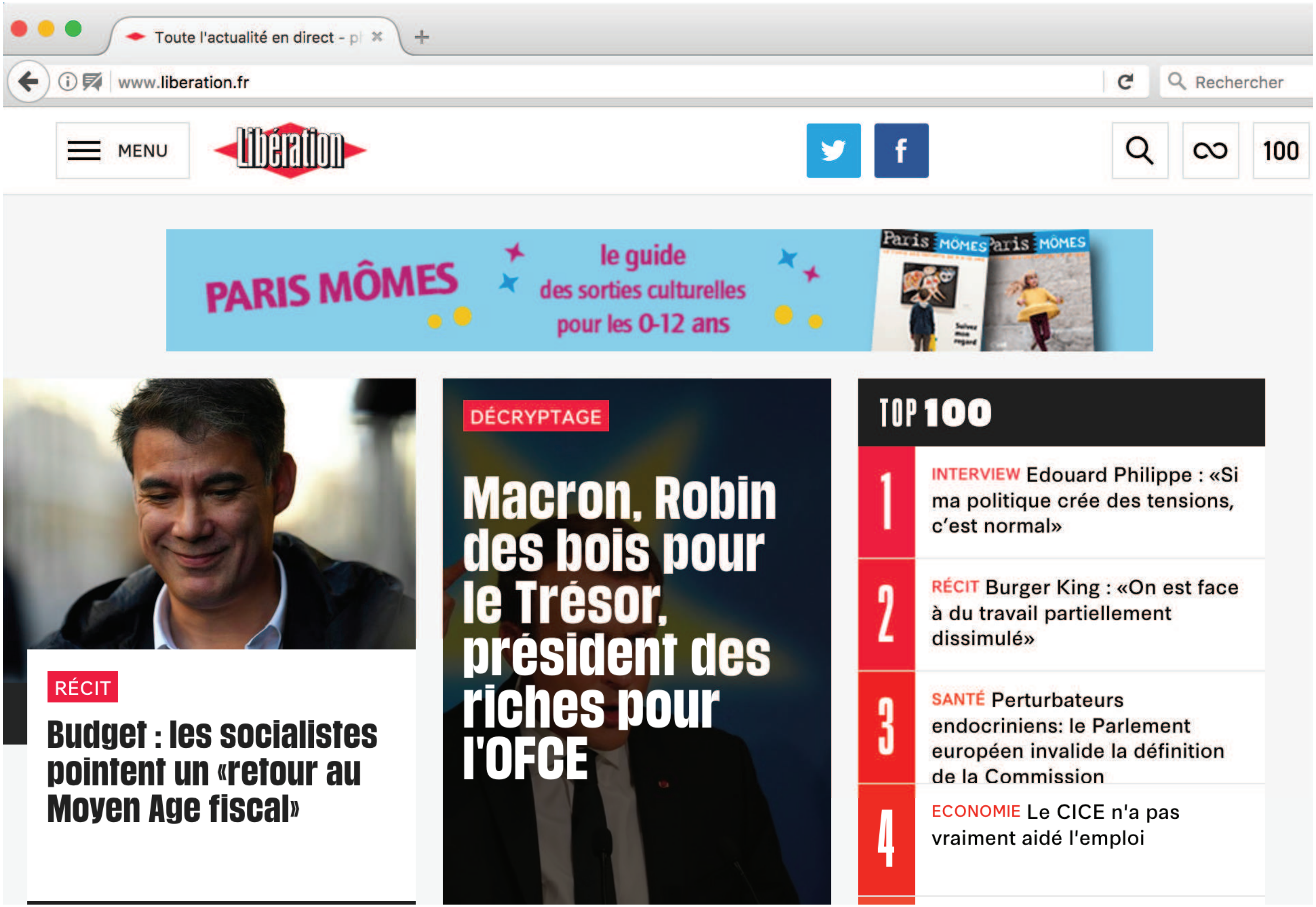
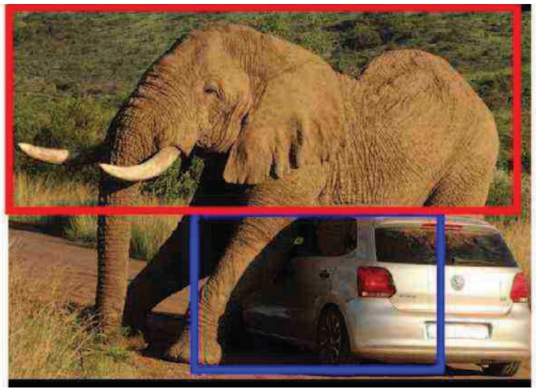
Machine learning for large-scale data

- **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.

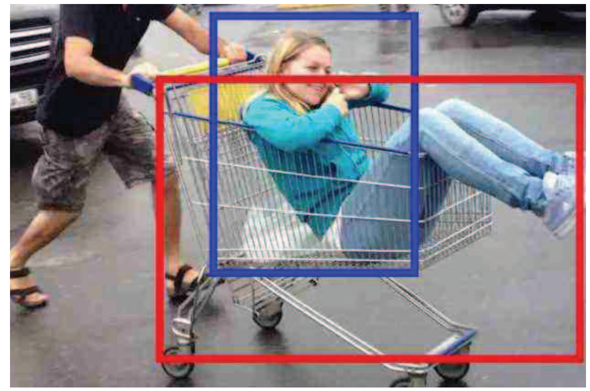
Advertising



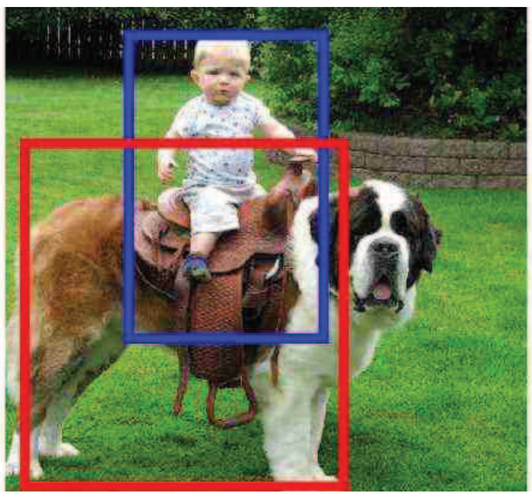
Object / action recognition in images



car under elephant



person in cart

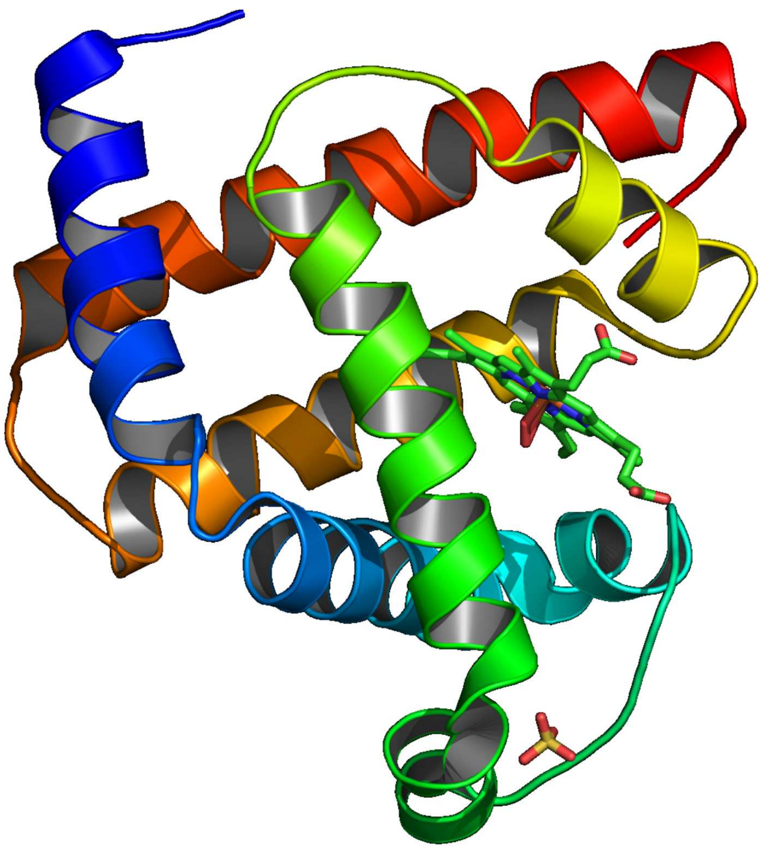


person ride dog

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

- **Ideal running-time complexity**: $O(dn)$

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- **Ideal running-time complexity**: $O(dn)$

- **Going back to simple methods**
  - Stochastic gradient methods (Robbins and Monro, 1951)

- **Goal: Present classical algorithms and some recent progress**

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

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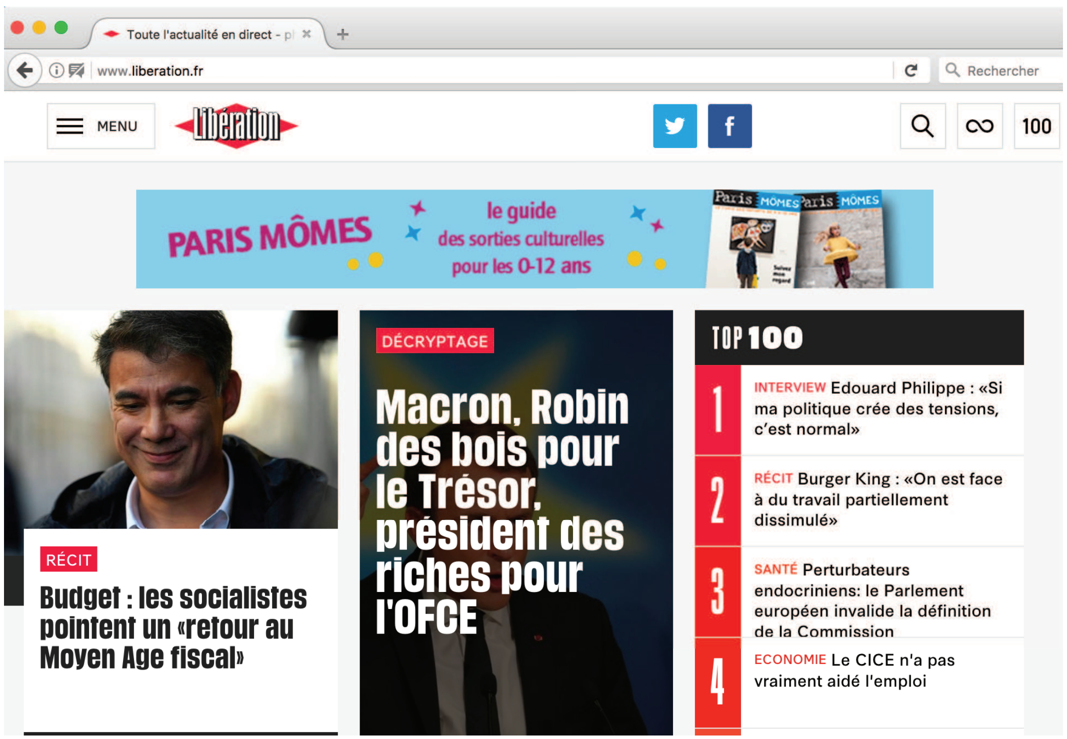

- **Advertising**: $n > 10^9$
  - $\Phi(x) \in \{0, 1\}^d$, $d > 10^9$
  - Navigation history + ad

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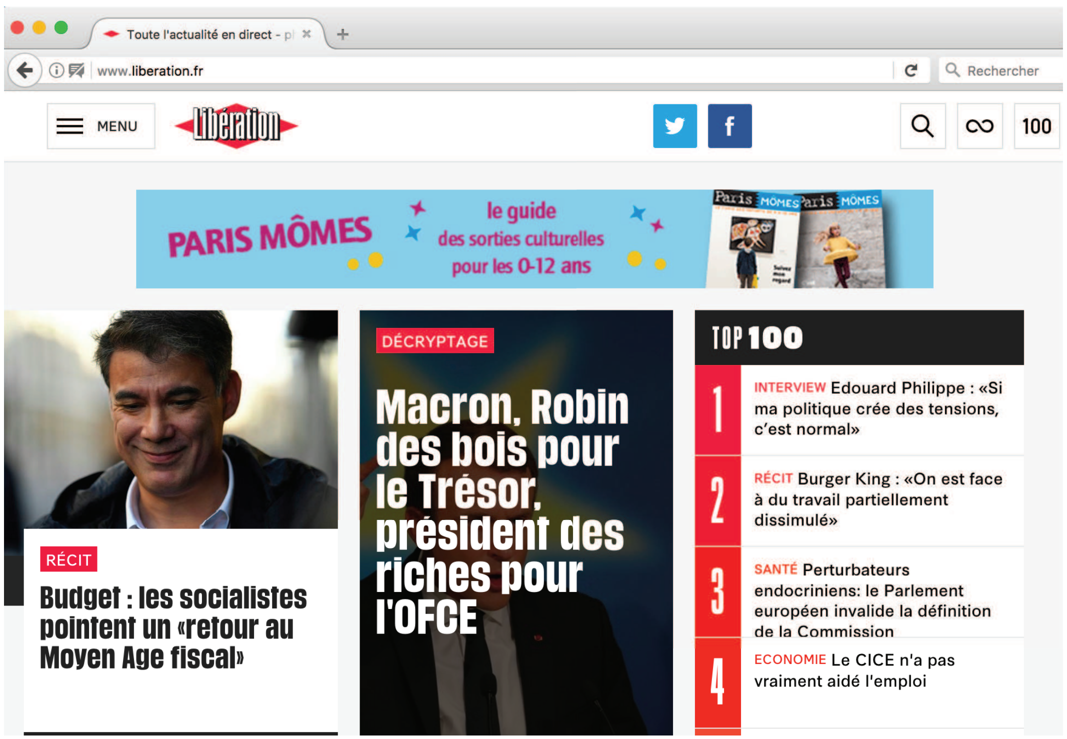

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- Linear predictions
  - $h(x, \theta) = \theta^\top \Phi(x)$

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x_1 $\quad$ x_2 $\quad$ x_3 $\quad$ x_4 $\quad$ x_5 $\quad$ x_6

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

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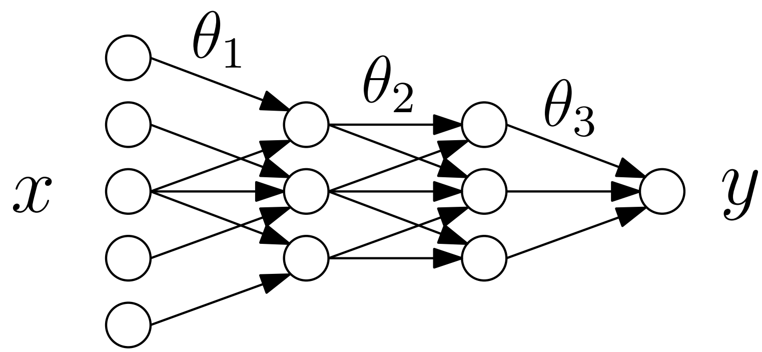
  – Neural networks $(n, d > 10^6)$: $h(x, \theta) = \theta_m^\top \sigma(\theta_{m-1}^\top \sigma(\cdots \theta_2^\top \sigma(\theta_1^\top x))$



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

data fitting term $+$ regularizer

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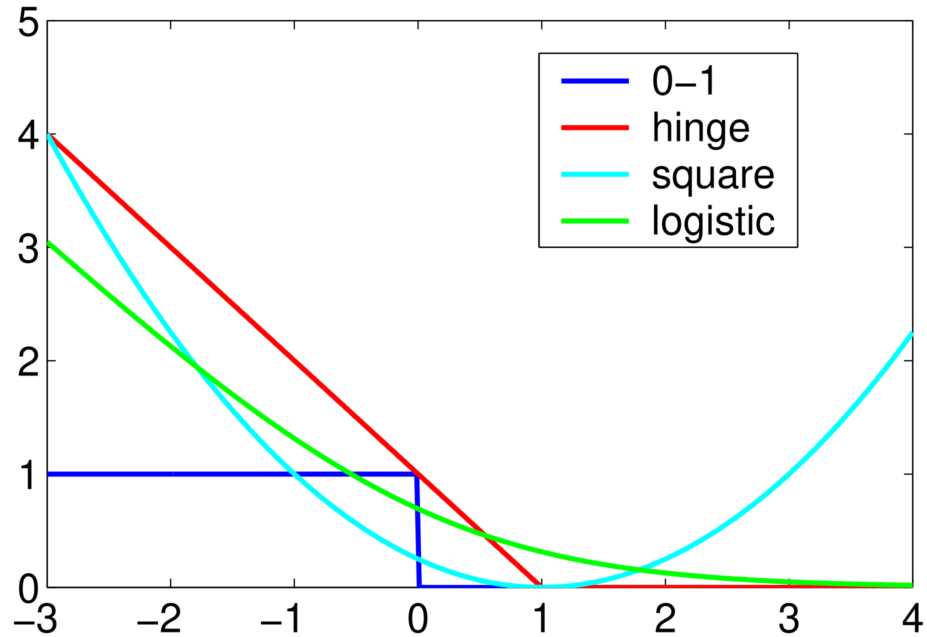
- **Classification** : $y \in \{-1,1\}$, prediction $\hat{y} = \text{sign}(h(x,\theta))$
  - loss of the form $\ell(y\,h(x,\theta))$
  - "True" 0-1 loss: $\ell(y\,h(x,\theta)) = 1_{y\,h(x,\theta)<0}$
  - Usual convex losses:



Main motivating examples

- **Support vector machine** (hinge loss): non-smooth

$$\ell(Y, h(X\theta)) = \max\{1 - Yh(X,\theta), 0\}$$

- **Logistic regression**: smooth

$$\ell(Y, h(X\theta)) = \log(1 + \exp(-Yh(X,\theta)))$$

- **Least-squares regression**

$$\ell(Y, h(X\theta)) = \frac{1}{2}(Y - h(X,\theta))^2$$

- **Structured output regression**
  - See Tsochantaridis et al. (2005); Lacoste-Julien et al. (2013)

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

- Optimization: optimization of regularized risk training cost

Parametric supervised machine learning

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

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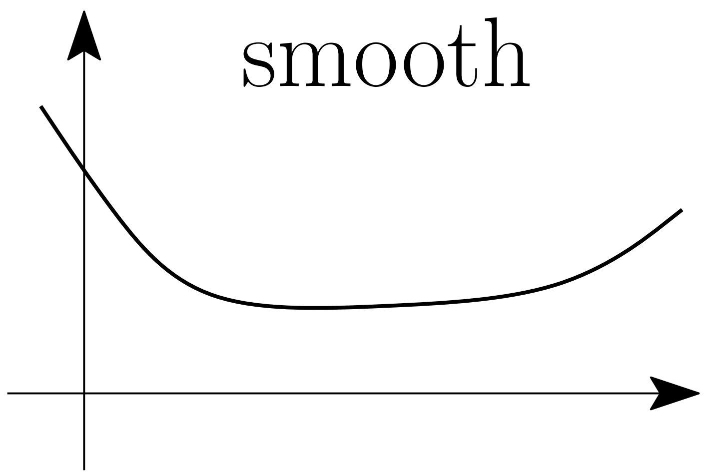
- Optimization: optimization of regularized risk training cost

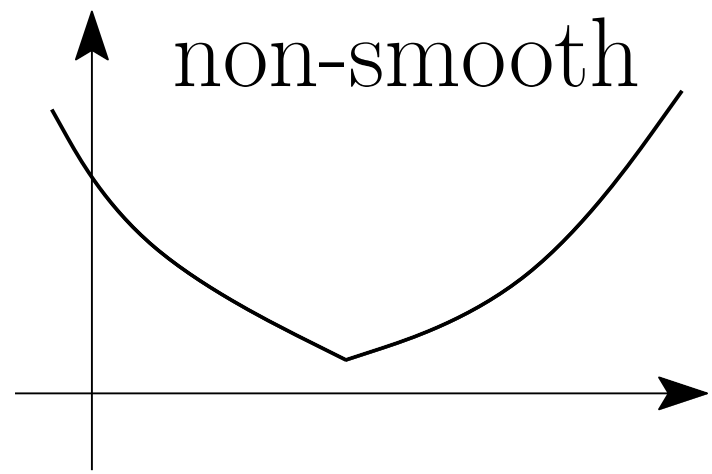
- Statistics: guarantees on $\mathbb{E}_{p(x,y)} \ell(y, h(x, \theta))$ testing cost

Smoothness and (strong) convexity

- A function $g : \mathbb{R}^d \rightarrow \mathbb{R}$ 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 board)*

Board

- Function $g(\theta) = \dfrac{1}{n} \sum_{i=1}^{n} \ell(y_i, \theta^\top \Phi(x_i))$

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- Gradient $g'(\theta) = \dfrac{1}{n} \displaystyle\sum_{i=1}^{n} \ell'(y_i, \theta^\top \Phi(x_i)) \Phi(x_i)$

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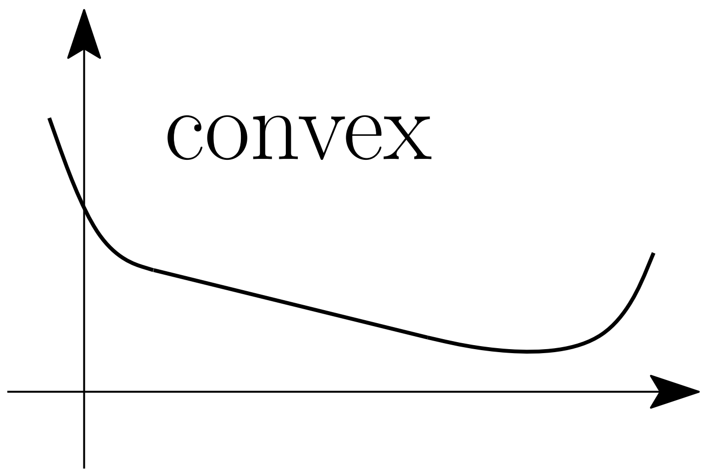
- Hessian $g''(\theta) = \dfrac{1}{n}\sum_{i=1}^{n} \ell''(y_i, \theta^\top \Phi(x_i))\Phi(x_i)\Phi(x_i)^\top$
  - Smooth loss $\Rightarrow \ell''(y_i, \theta^\top \Phi(x_i))$ bounded

Smoothness and (strong) convexity

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

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



Smoothness and (strong) convexity

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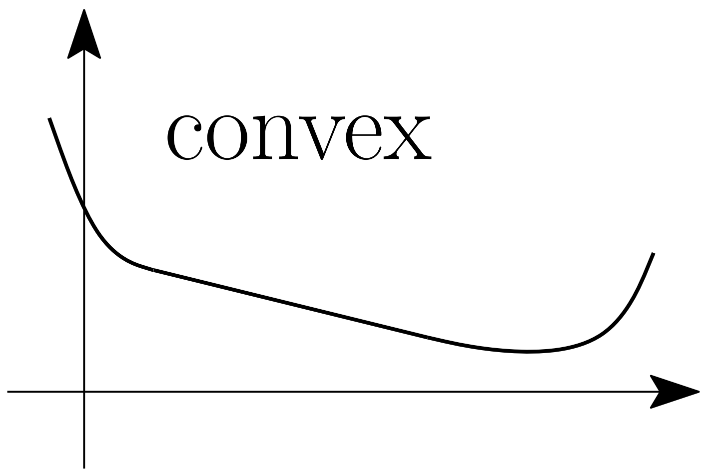

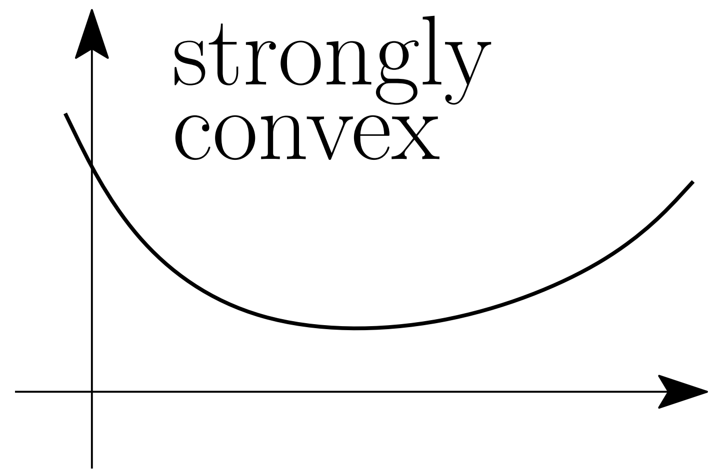

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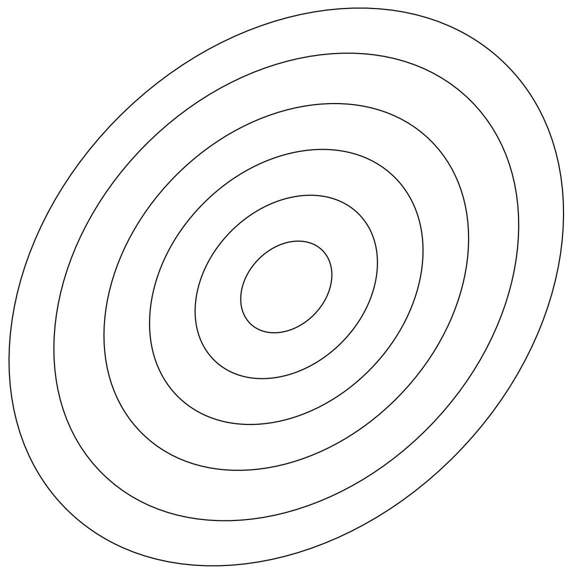
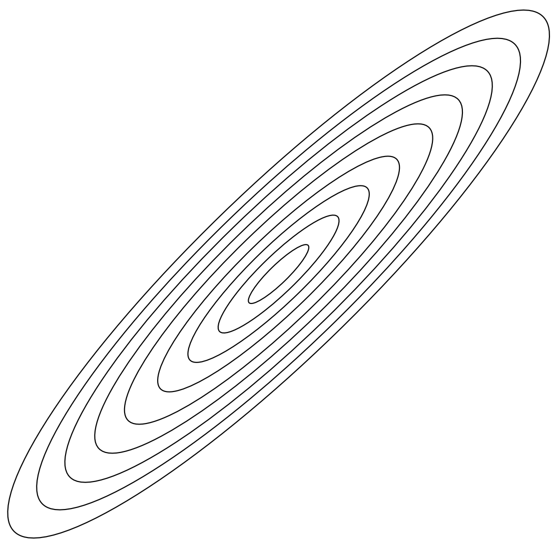
  – Condition number $\kappa = L/\mu \geqslant 1$



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

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  - 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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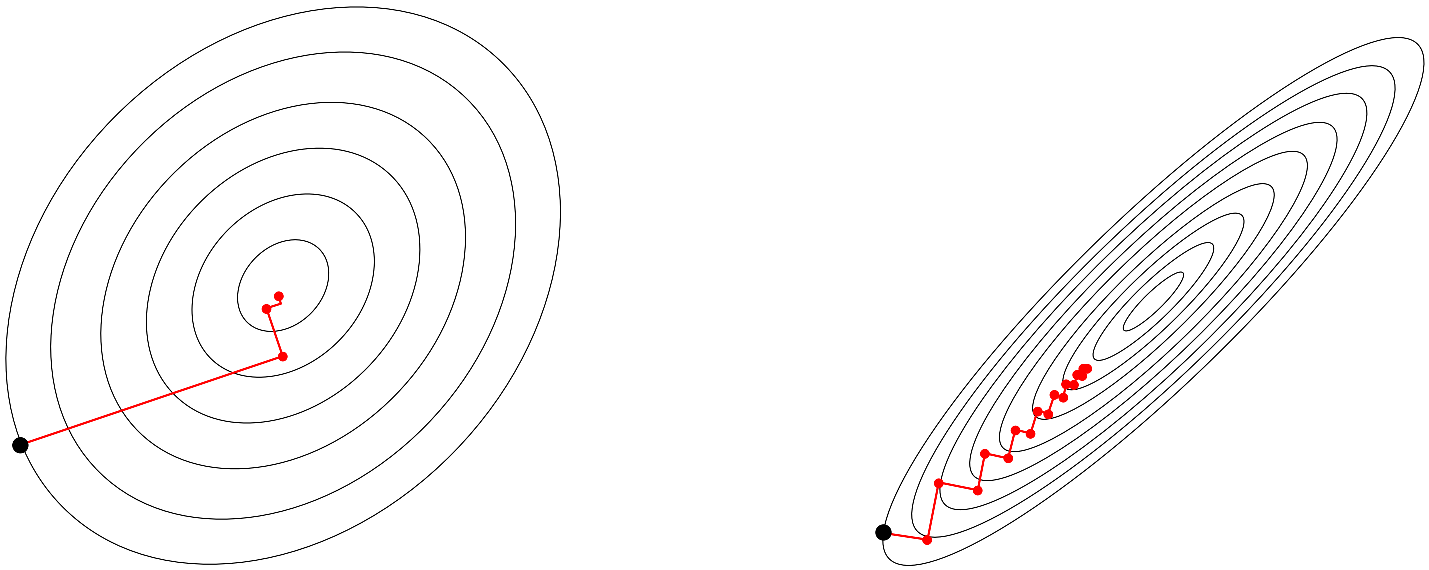
  - Even when $\mu > 0$, μ may be arbitrarily small!

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

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)*



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

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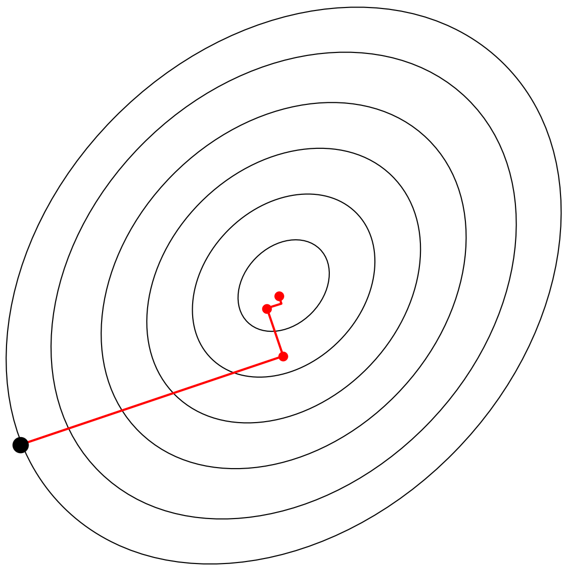
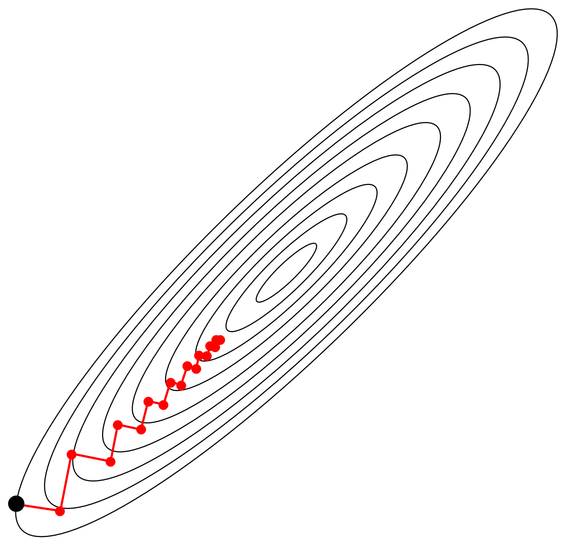
  $g(\theta_t) - g(\theta_*) \leqslant O(1/t)$

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



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



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

Gradient descent - Proof for quadratic functions

- Quadratic convex function: $g(\theta) = \frac{1}{2}\theta^\top H\theta - c^\top\theta$
  - μ and L are the smallest and largest eigenvalues of H
  - Global optimum $\theta_* = H^{-1}c$ (or $H^\dagger c$) such that $H\theta_* = c$

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\theta_t &= \theta_{t-1} - \frac{1}{L}(H\theta_{t-1} - c) = \theta_{t-1} - \frac{1}{L}(H\theta_{t-1} - H\theta_*) \\
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- **Strong convexity** $\mu > 0$: eigenvalues of $(I - \frac{1}{L}H)^t$ in $[0, (1 - \frac{\mu}{L})^t]$
  - Convergence of iterates: $\|\theta_t - \theta_*\|^2 \leqslant (1 - \mu/L)^{2t}\|\theta_0 - \theta_*\|^2$
  - Function values: $g(\theta_t) - g(\theta_*) \leqslant (1 - \mu/L)^{2t}\big[g(\theta_0) - g(\theta_*)\big]$

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- **Convexity** $\mu = 0$: eigenvalues of $(I - \frac{1}{L}H)^t$ in $[0, 1]$
  - No convergence of iterates: $\|\theta_t - \theta_*\|^2 \leqslant \|\theta_0 - \theta_*\|^2$
  - Function values: $g(\theta_t) - g(\theta_*) \leqslant \max_{v\in[0,L]} v(1 - v/L)^{2t}\|\theta_0 - \theta_*\|^2$

    $g(\theta_t) - g(\theta_*) \leqslant \frac{L}{t}\|\theta_0 - \theta_*\|^2$ *(board)*

Board

- No convergence of iterates: $\|\theta_t - \theta_*\|^2 \leqslant \|\theta_0 - \theta_*\|^2$

- $g(\theta_t) - g(\theta_*) = \frac{1}{2}(\theta_t - \theta_*)^\top H(\theta_t - \theta_*)$, which is equal to

$$\frac{1}{2}(\theta_0 - \theta_*)^\top H(I - \frac{1}{L}H)^{2t}(\theta_0 - \theta_*)$$

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$$\begin{aligned} v(1 - v/L)^{2t} &\leqslant v \exp(-v/L)^{2t} = v \exp(-2tv/L) \\ &\leqslant (2tv/L) \exp(-2tv/L) \times \frac{L}{2t} \\ &\leqslant \max_{\alpha \geqslant 0} \alpha \exp(-\alpha) \times \frac{L}{2t} = O(\frac{L}{2t}) \end{aligned}$$

Iterative methods for minimizing smooth functions

- **Assumption**: g convex and L-smooth on $\mathbb{R}^d$

- **Gradient descent**: $\theta_t = \theta_{t-1} - \gamma_t \, g'(\theta_{t-1})$
  - $O(1/t)$ convergence rate for convex functions
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  - $O\big(e^{-\rho 2^t}\big)$ *quadratic* rate *(see board)*

Board

- Second-order Taylor expansion

$$g(\theta) \approx g(\theta_{t-1}) + g'(\theta_{t-1})^\top(\theta - \theta_{t-1}) + \frac{1}{2}(\theta - \theta_{t-1})^\top g''(\theta_{t-1})(\theta - \theta_{t-1})$$

  – Minimization by zeroing gradient:

$$g'(\theta_{t-1}) + g''(\theta_{t-1})(\theta - \theta_{t-1}) = 0$$

  – Iteration: $\theta_t = \theta_{t-1} - g''(\theta_{t-1})^{-1} g'(\theta_{t-1})$

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  1. No need to optimize below statistical error
  2. Cost functions are averages
  3. Testing error is more important than training error

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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
   - Constant step-sizes: 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 $(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}$, $i = 1, \dots, n$, **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 $\{1, \dots, n\}$
  - Polyak-Ruppert averaging: $\bar{\theta}_t = \frac{1}{t+1} \sum_{u=0}^{t} \theta_u$

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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: $O(d \cdot \kappa/\varepsilon)$

Impact of averaging (Bach and Moulines, 2011)

- Stochastic gradient descent with learning rate $\gamma_t = Ct^{-\alpha}$

- **Strongly convex smooth objective functions**
  - Non-asymptotic analysis with explicit constants
  - Forgetting of initial conditions
  - Robustness to the choice of C

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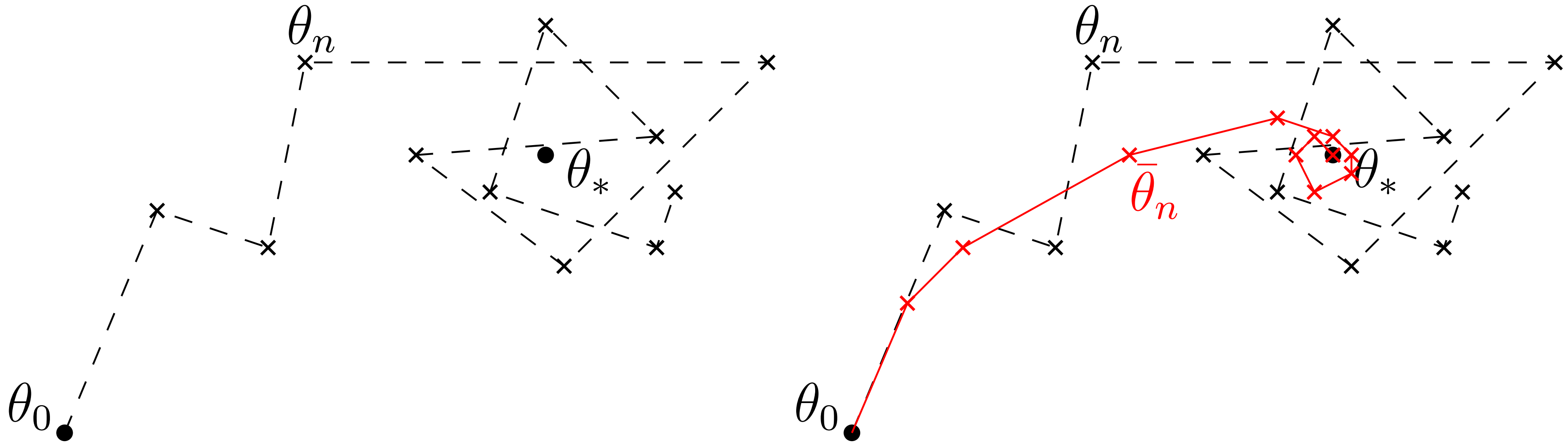
- **Strongly convex smooth objective functions**
  - Non-asymptotic analysis with explicit constants
  - Forgetting of initial conditions
  - Robustness to the choice of C
- **Convergence rates** for $\mathbb{E}\|\theta_t - \theta_*\|^2$ and $\mathbb{E}\|\bar{\theta}_t - \theta_*\|^2$
  - no averaging: $O\Big(\frac{\sigma^2\gamma_t}{\mu}\Big) + O(e^{-\mu t \gamma_t})\|\theta_0 - \theta_*\|^2$
  - averaging: $\frac{\operatorname{tr} H(\theta_*)^{-1}}{t} + O\Big(\frac{\|\theta_0 - \theta_*\|^2}{\mu^2 t^2}\Big)$

    (see board)

Board

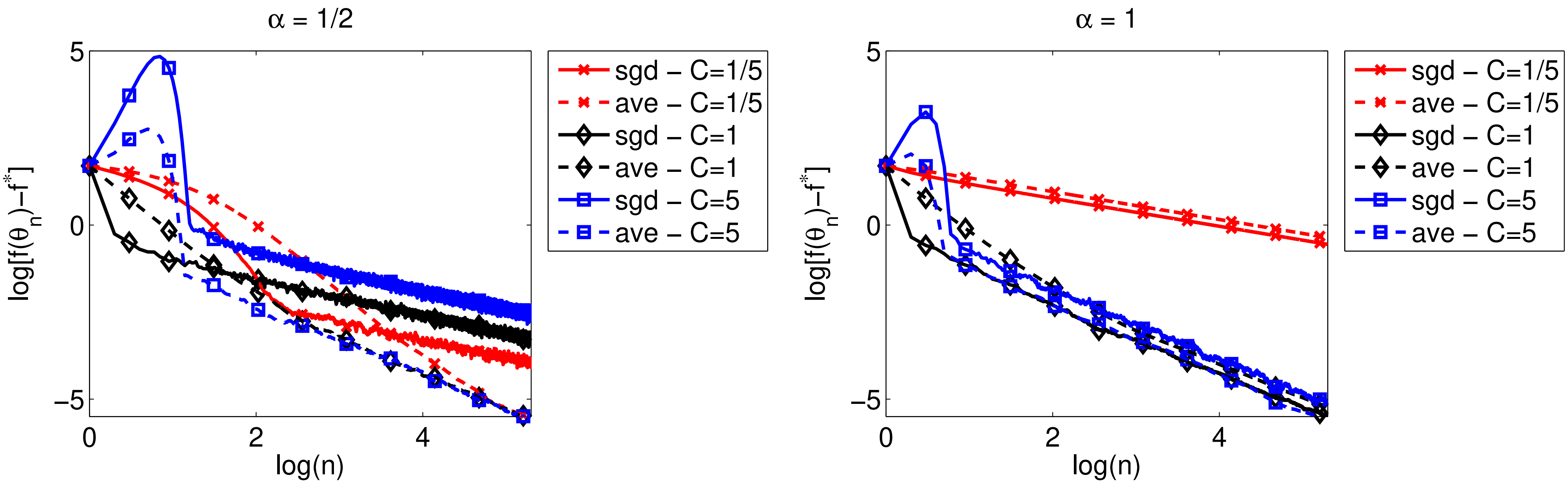
- Leaving initial point θ_0 to reach θ_*

- Impact of averaging



Robustness to wrong constants for $\gamma_t = Ct^{-\alpha}$

- $f(\theta) = \frac{1}{2}|\theta|^2$ with i.i.d. Gaussian noise ($d = 1$)
- Left: $\alpha = 1/2$
- Right: $\alpha = 1$



- See also `http://leon.bottou.org/projects/sgd`

Stochastic vs. deterministic methods

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

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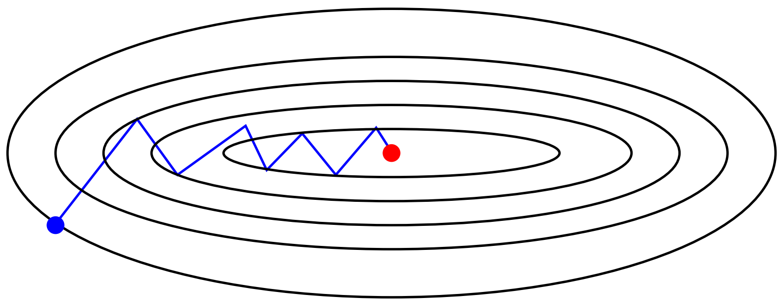

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  - Convergence rate in $O(\kappa/t)$
  - Iteration complexity is independent of n

Stochastic vs. deterministic methods

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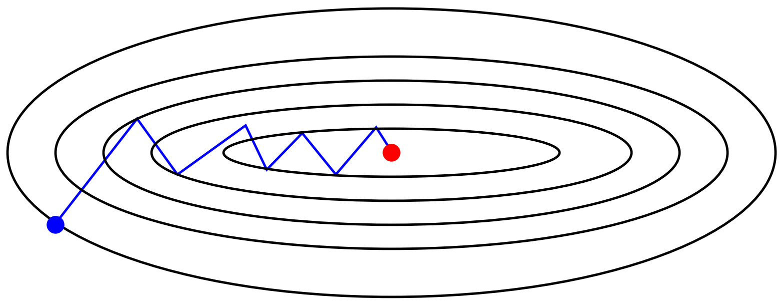

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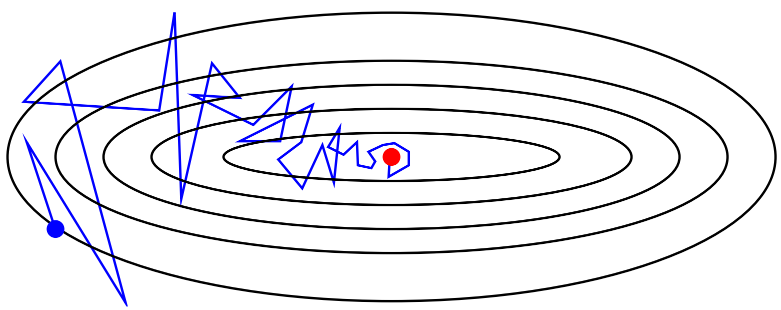

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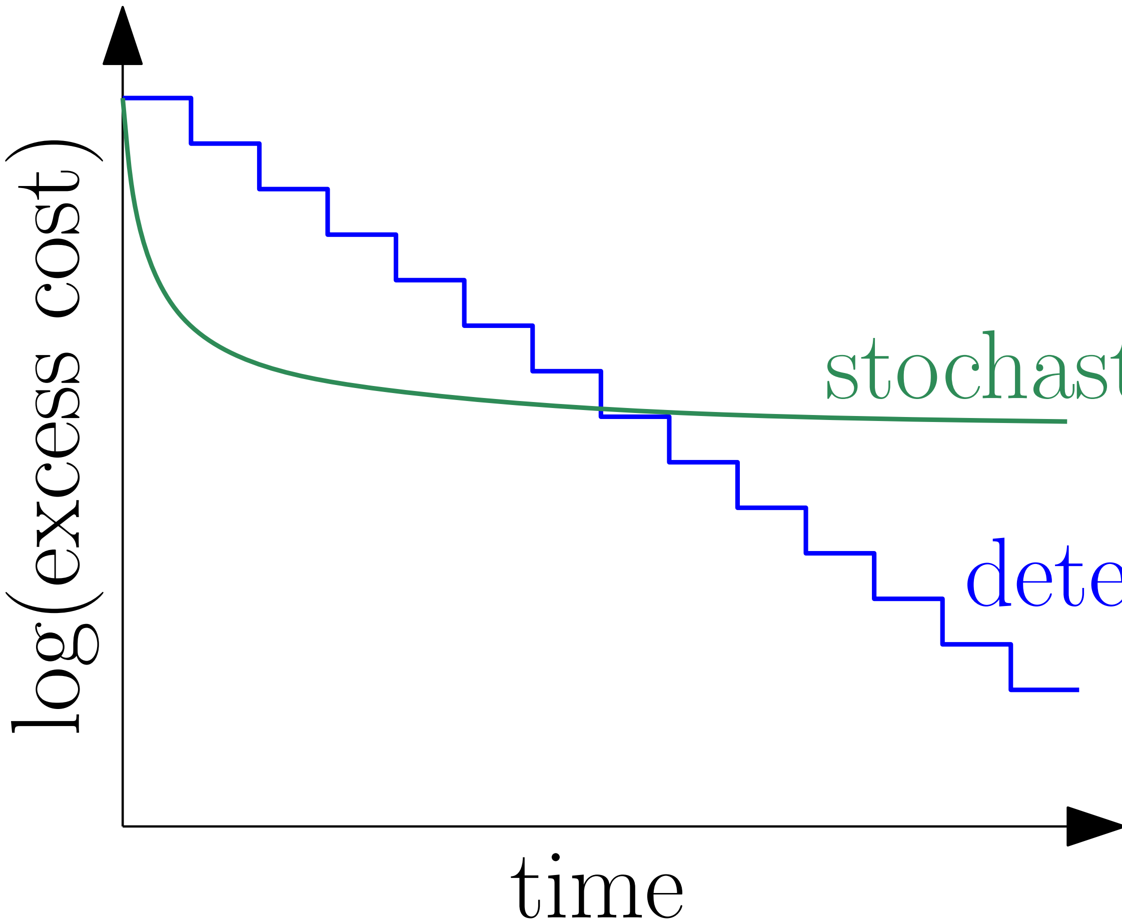
- **Goal = best of both worlds**: Linear rate with $O(d)$ iteration cost
  Simple choice of step size



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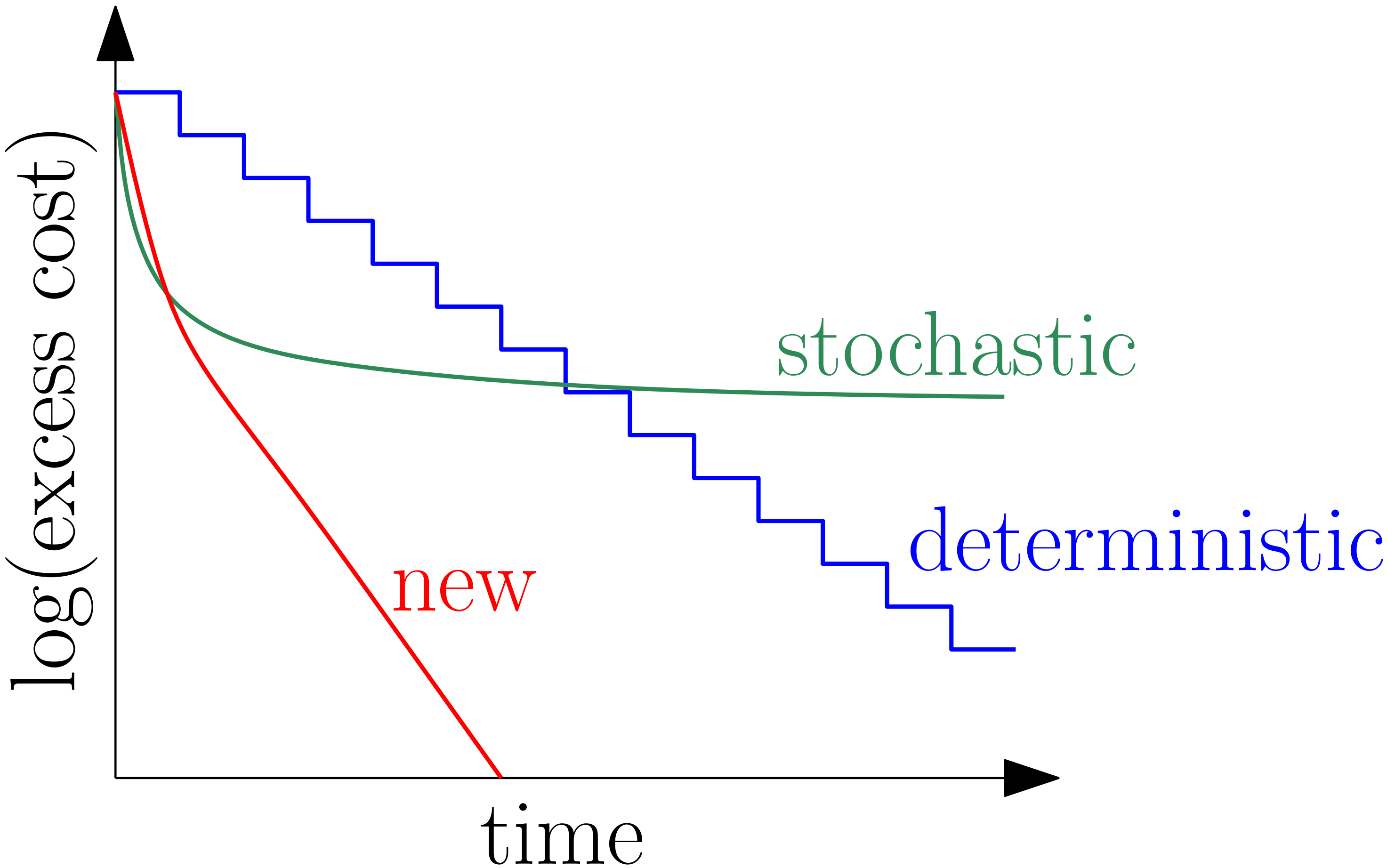

Accelerating gradient methods - Related work

- **Generic acceleration** (Nesterov, 1983, 2004)

$$\theta_t = \eta_{t-1} - \gamma_t g'(\eta_{t-1}) \text{ and } \eta_t = \theta_t + \delta_t(\theta_t - \theta_{t-1})$$

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  – Still $O(nd)$ iteration cost: complexity $= O(nd \cdot \sqrt{\kappa} \log \frac{1}{\varepsilon})$

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- **Constant step-size stochastic gradient**
  - Solodov (1998); Nedic and Bertsekas (2000)
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- **Stochastic version of accelerated batch gradient methods**
  - Tseng (1998); Ghadimi and Lan (2010); Xiao (2010)
  - Can improve constants, but still have sublinear $O(1/t)$ rate

Stochastic average gradient (Le Roux, Schmidt, and Bach, 2012)

- **Stochastic average gradient** (SAG) iteration
  - Keep in memory the gradients of all functions f_i, $i = 1, \dots, n$
  - Random selection $i(t) \in \{1, \dots, n\}$ with replacement
  - Iteration: $\theta_t = \theta_{t-1} - \frac{\gamma_t}{n} \sum_{i=1}^{n} y_i^t$ with $y_i^t = \begin{cases} f_i'(\theta_{t-1}) & \text{if } i = i(t) \\ y_i^{t-1} & \text{otherwise} \end{cases}$

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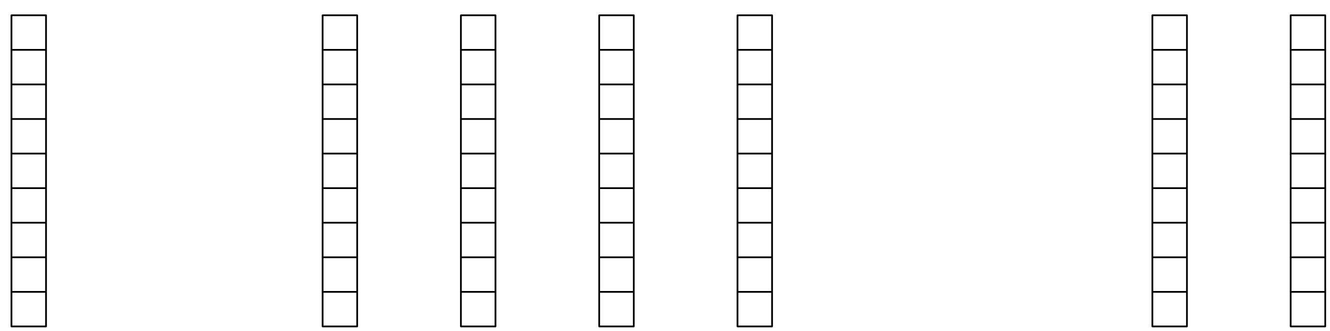

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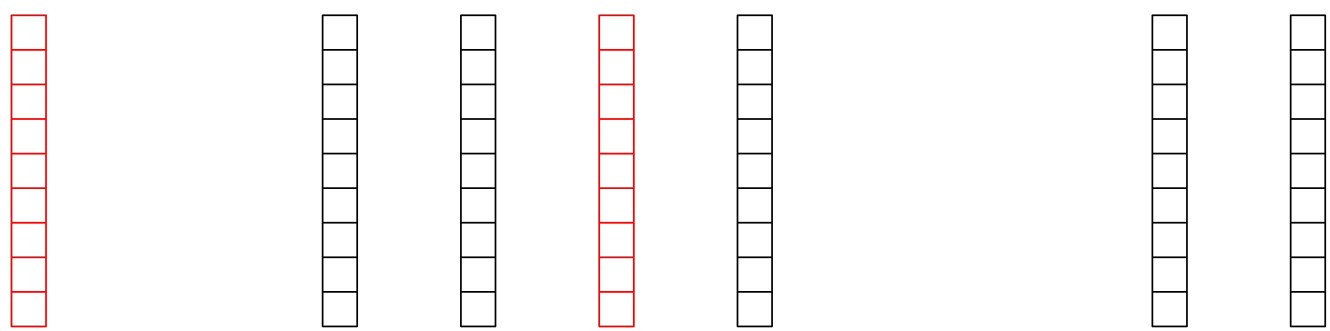

Stochastic average gradient
(Le Roux, Schmidt, and Bach, 2012)

- **Stochastic average gradient** (SAG) iteration
  - Keep in memory the gradients of all functions f_i, $i = 1, \dots, n$
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functions	$g = \frac{1}{n}\sum_{i=1}^n f_i$	f_1	f_2	f_3	f_4	$\bullet\bullet\bullet$	f_{n-1}	f_n
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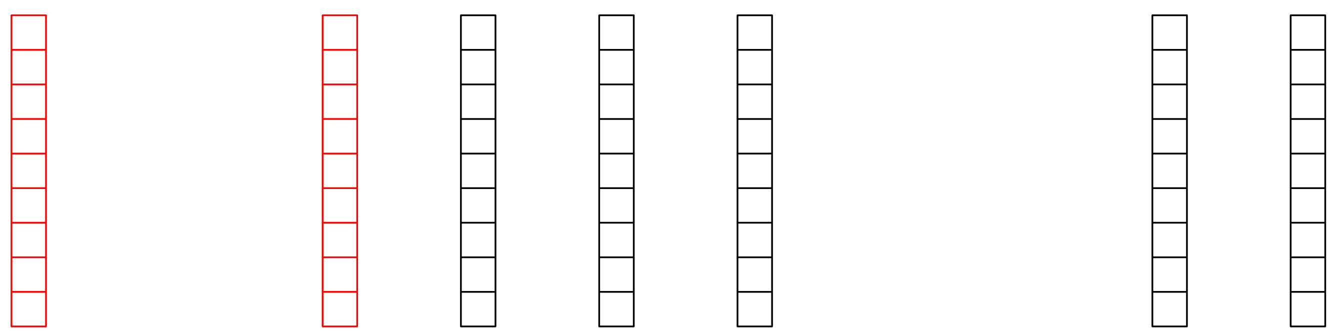

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- Stochastic version of incremental average gradient (Blatt et al., 2008)

- **Extra memory requirement**: n gradients in $\mathbb{R}^d$ in general

- **Linear supervised machine learning**: only n real numbers
  - If $f_i(\theta) = \ell(y_i, \Phi(x_i)^\top \theta)$, then $f_i'(\theta) = \ell'(y_i, \Phi(x_i)^\top \theta)\, \Phi(x_i)$

Running-time comparisons (strongly-convex)

- **Assumptions**: $g(\theta) = \frac{1}{n}\sum_{i=1}^n f_i(\theta)$
  - Each f_i convex L-smooth and g μ-strongly convex, $\kappa = L/\mu$

Stochastic gradient descent	$d\times \quad \frac{L}{\mu} \quad \times \quad \frac{1}{\varepsilon}$
Gradient descent	$d\times \quad n\frac{L}{\mu} \quad \times \log\frac{1}{\varepsilon}$
Accelerated gradient descent	$d\times \quad n\sqrt{\frac{L}{\mu}} \quad \times \log\frac{1}{\varepsilon}$
SAG	$d\times \quad (n + \frac{L}{\mu}) \quad \times \log\frac{1}{\varepsilon}$

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

Running-time comparisons (non-strongly-convex)

- **Assumptions**: $g(\theta) = \frac{1}{n}\sum_{i=1}^{n} f_i(\theta)$
  - Each f_i convex L-smooth
  - Ill conditioned problems: g may not be strongly-convex ($\mu = 0$)

Stochastic gradient descent	$d\times$	$1/\varepsilon^2$
Gradient descent	$d\times$	n/ε
Accelerated gradient descent	$d\times$	$n/\sqrt{\varepsilon}$
SAG	$d\times$	$\sqrt{n}/\varepsilon$

- Adaptivity to potentially hidden strong convexity

- No need to know the local/global strong-convexity constant

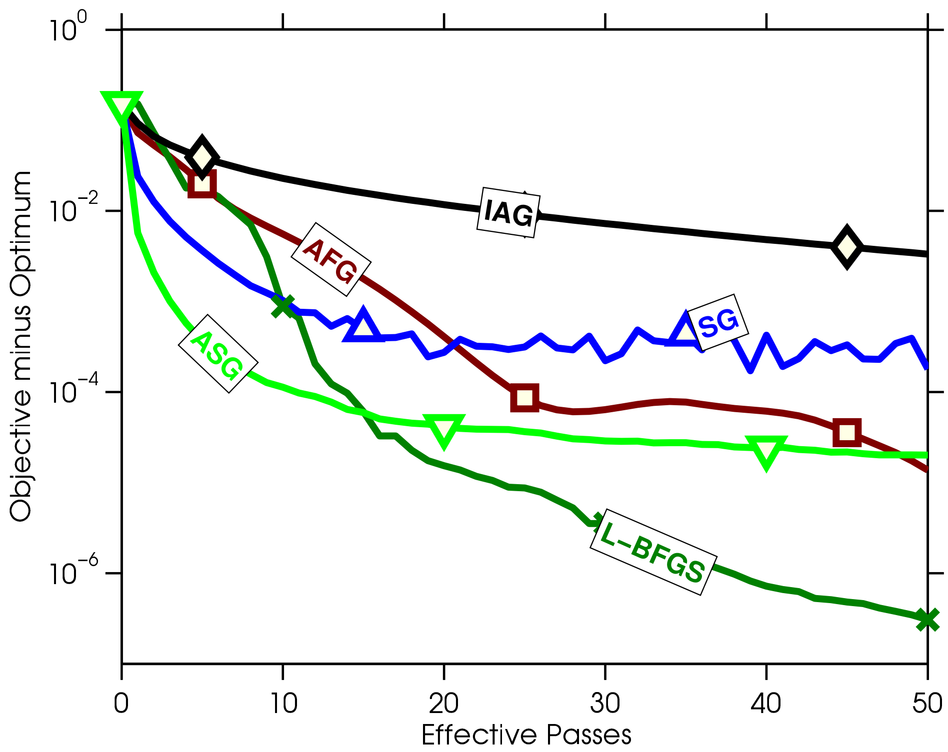
Stochastic average gradient
Implementation details and extensions

- **Sparsity in the features**
  - Just-in-time updates $\Rightarrow$ replace $O(d)$ by number of non zeros
  - See also Leblond, Pedregosa, and Lacoste-Julien (2016)
- **Mini-batches**
  - Reduces the memory requirement $+$ block access to data
- **Line-search**
  - Avoids knowing L in advance
- **Non-uniform sampling**
  - Favors functions with large variations
- See `www.cs.ubc.ca/~schmidtm/Software/SAG.html`

Experimental results (logistic regression)

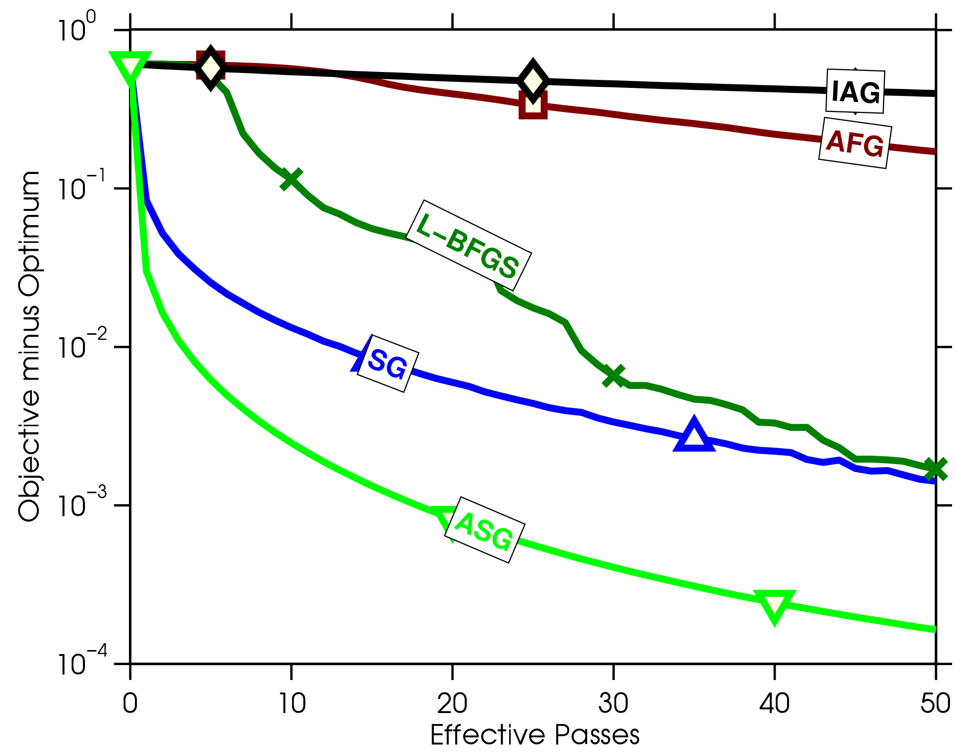
quantum dataset

$(n = 50\ 000,\ d = 78)$



rcv1 dataset

$(n = 697\ 641,\ d = 47\ 236)$



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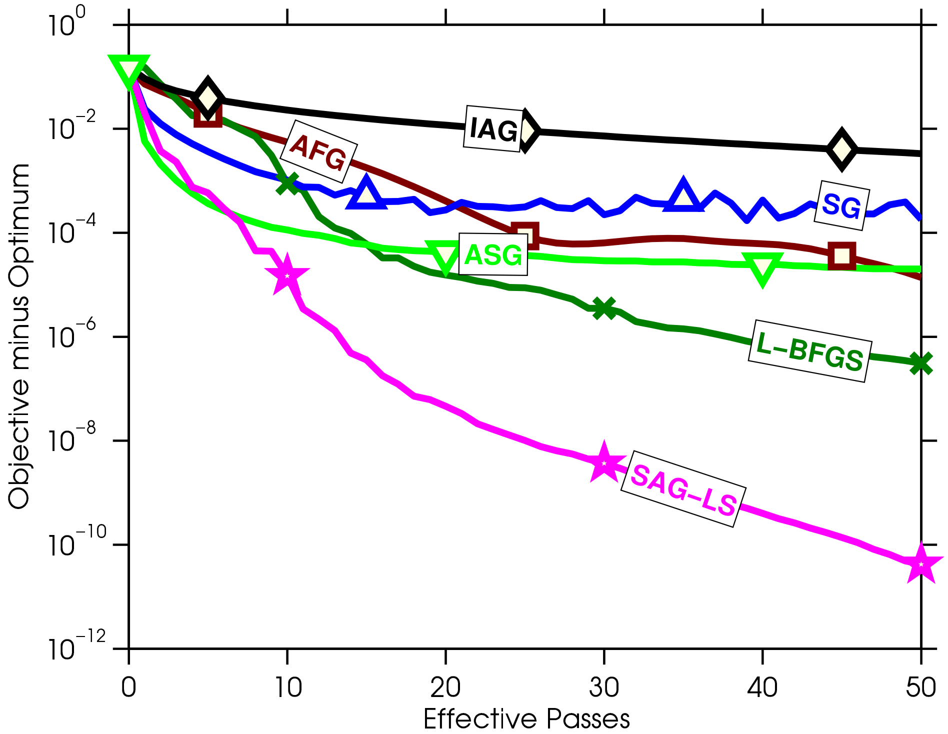

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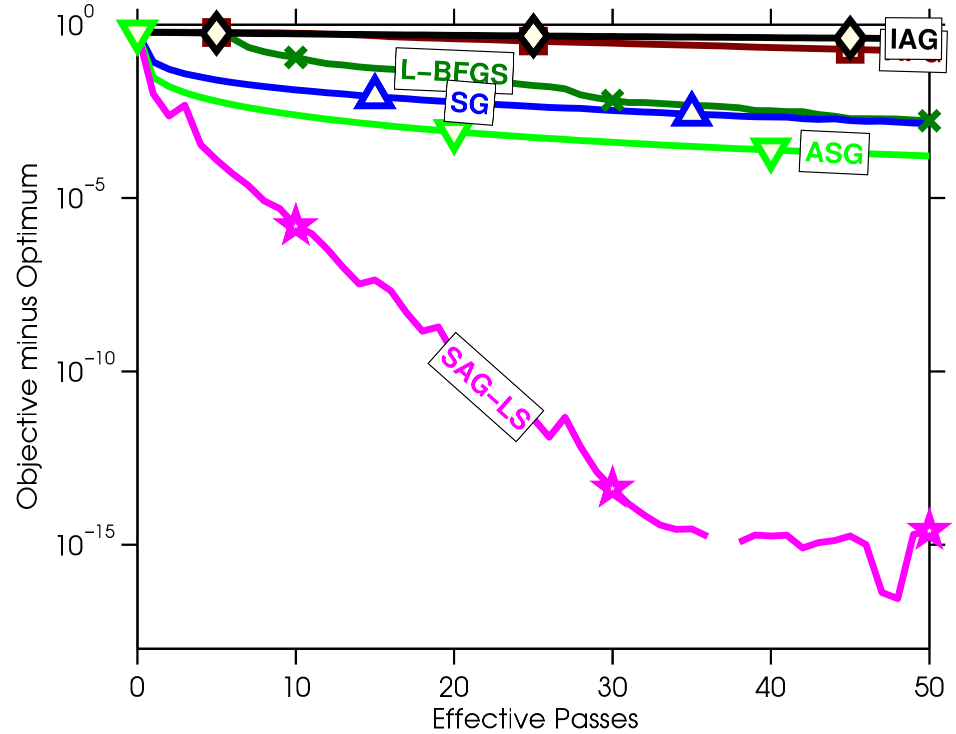
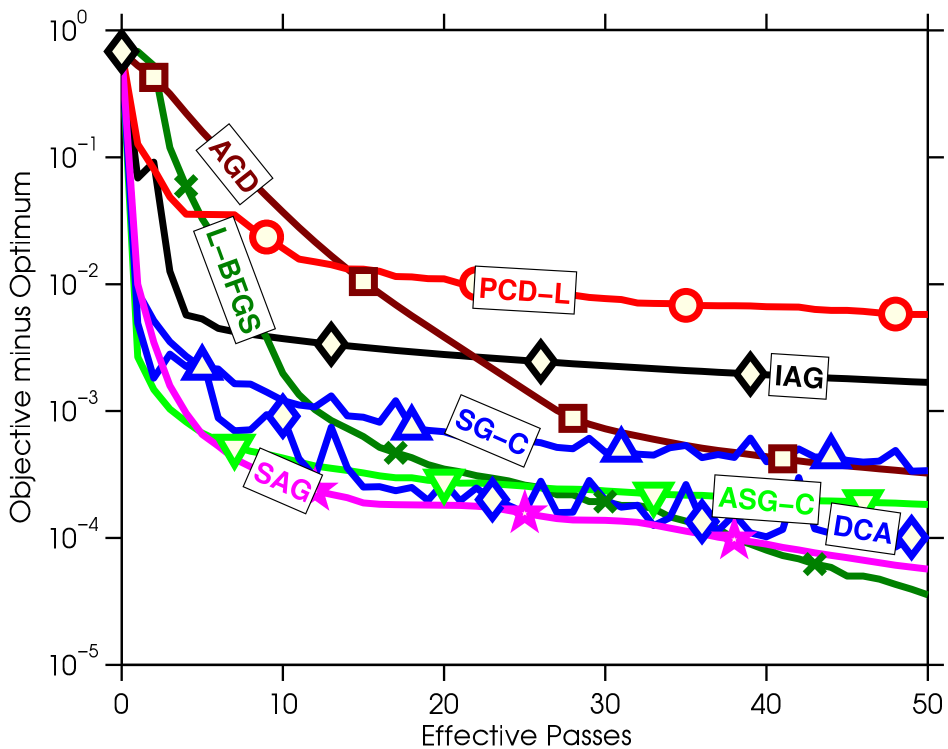
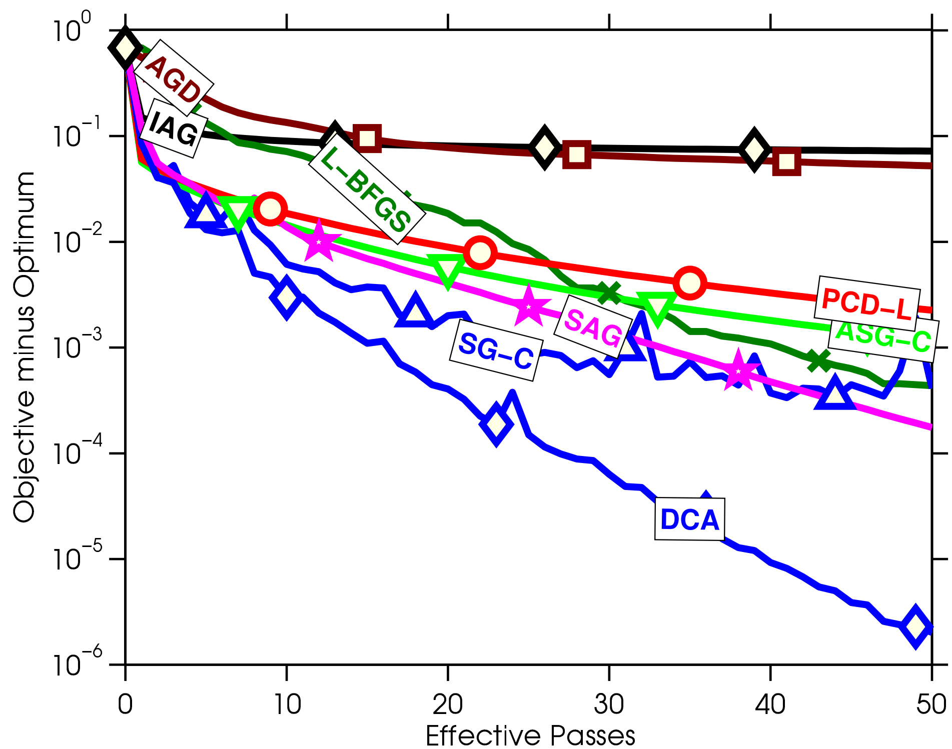


Before non-uniform sampling

protein dataset
$(n = 145\ 751,\ d\ = 74)$



sido dataset
$(n = 12\ 678,\ d = 4\ 932)$



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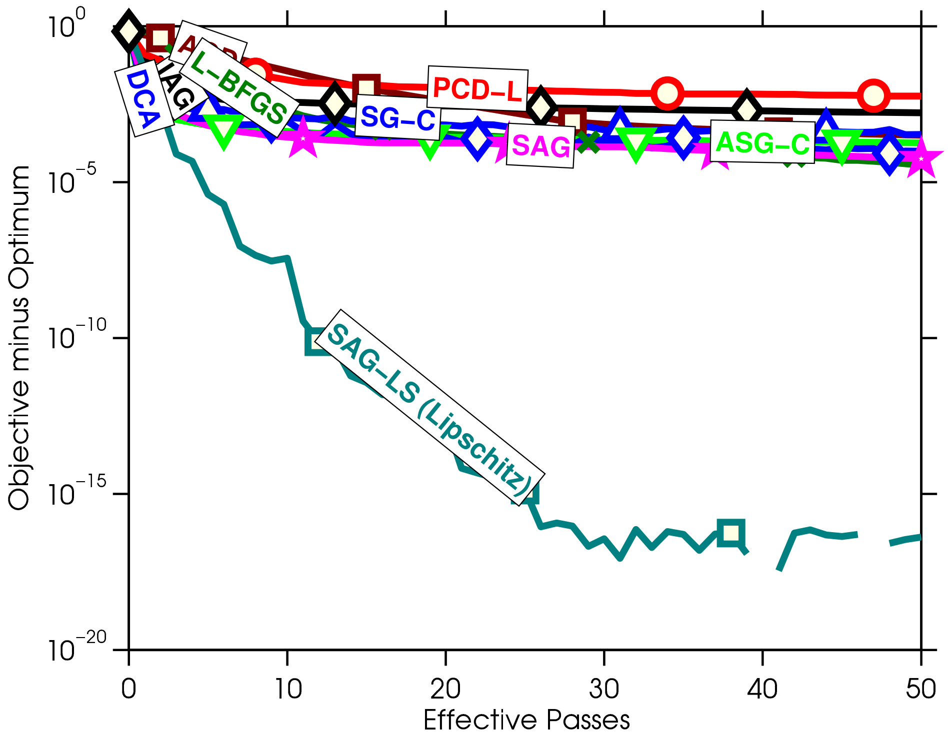

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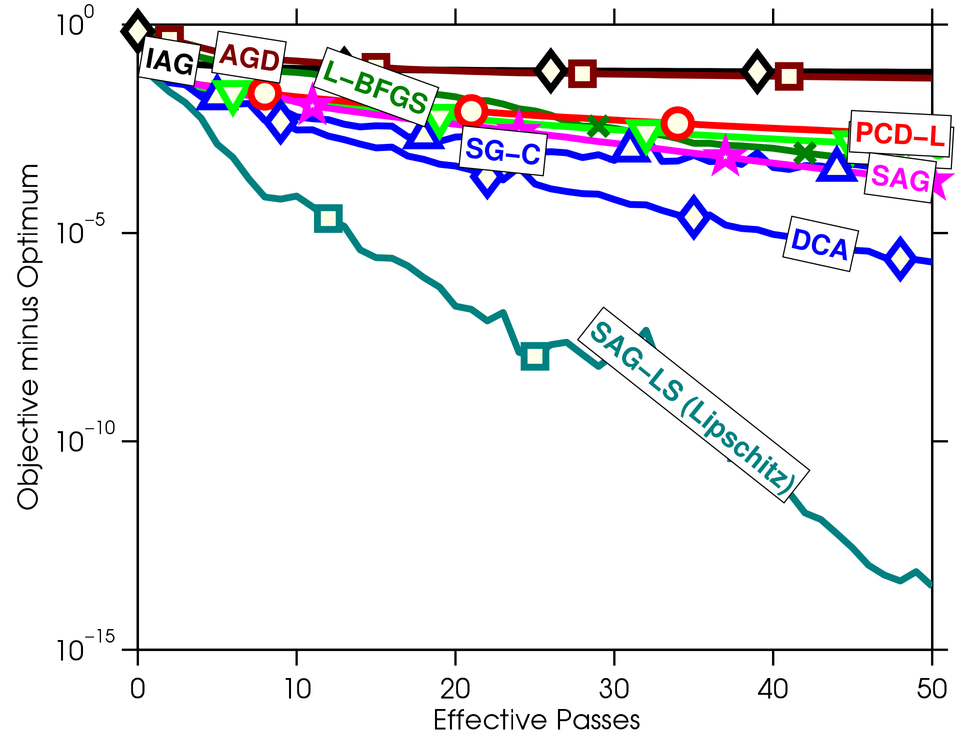
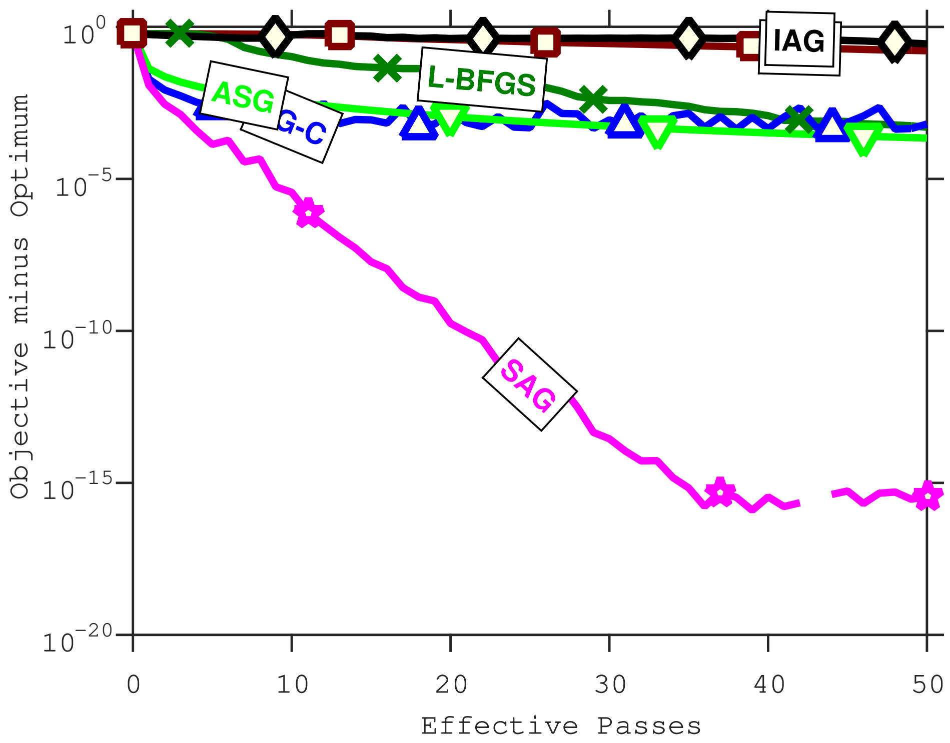


From training to testing errors

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

Training cost



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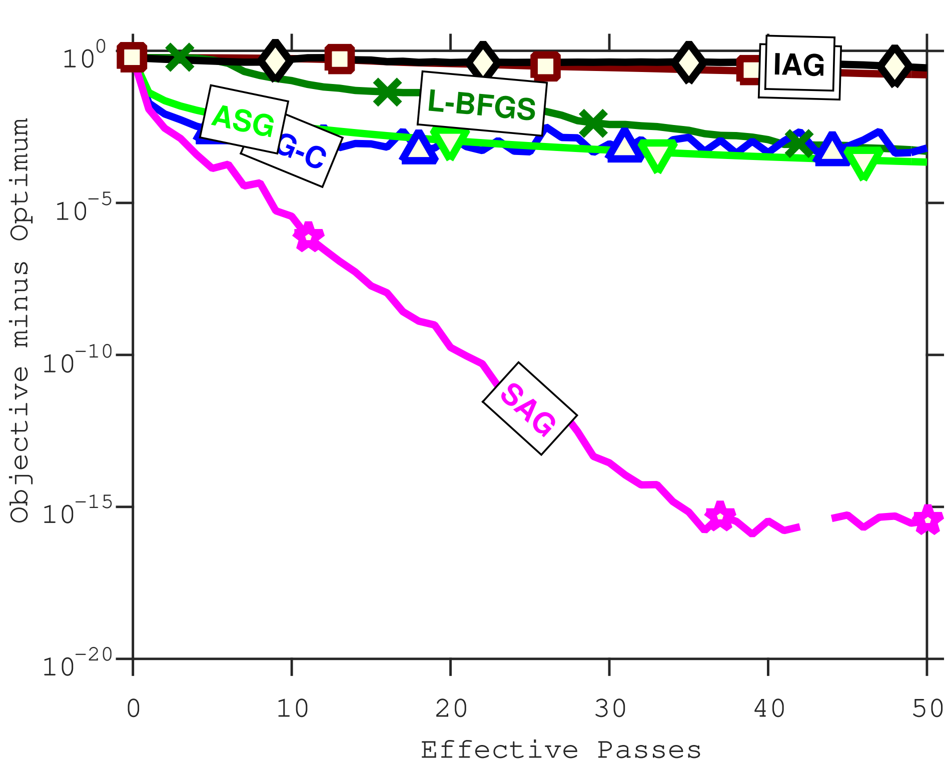
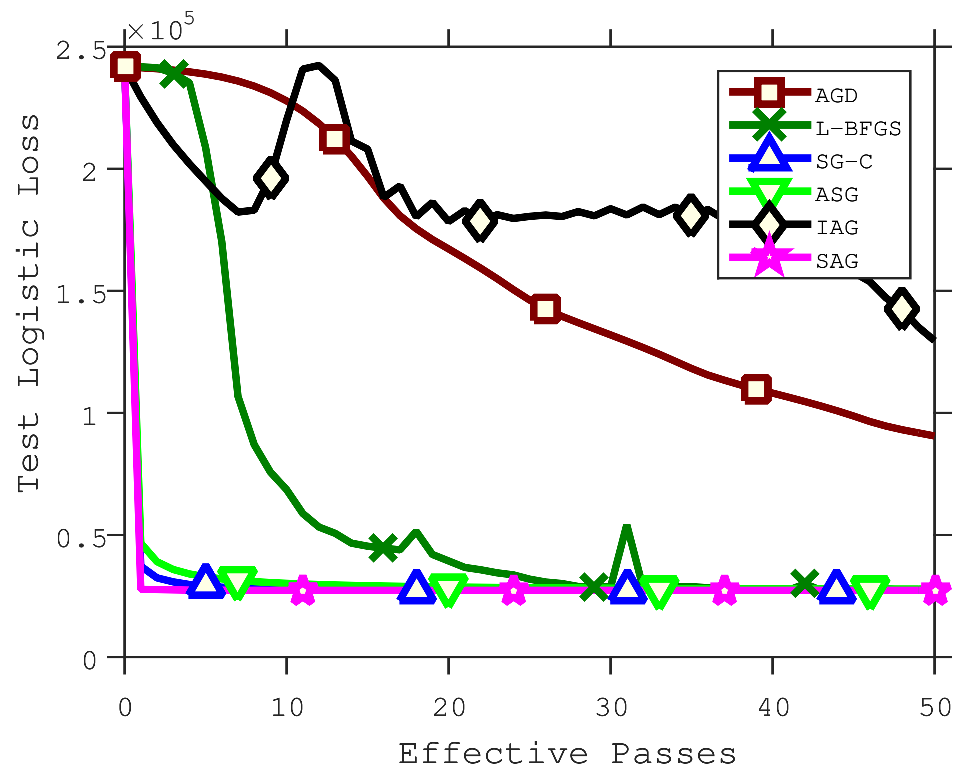


Testing cost



Linearly convergent stochastic gradient algorithms

- **Many related algorithms**
  - SAG (Le Roux, Schmidt, and Bach, 2012)
  - SDCA (Shalev-Shwartz and Zhang, 2013)
  - SVRG (Johnson and Zhang, 2013; Zhang et al., 2013)
  - MISO (Mairal, 2015)
  - Finito (Defazio et al., 2014b)
  - SAGA (Defazio, Bach, and Lacoste-Julien, 2014a)
  - ...

- **Similar rates of convergence and iterations**

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- **Similar rates of convergence and iterations**

- **Different interpretations and proofs / proof lengths**
  - Lazy gradient evaluations
  - Variance reduction

Acceleration

- **Similar guarantees for finite sums**: SAG, SDCA, SVRG (Xiao and Zhang, 2014), SAGA, MISO (Mairal, 2015)

Gradient descent	$d\times$	$n\frac{L}{\mu}$	$\times \log\frac{1}{\varepsilon}$
Accelerated gradient descent	$d\times$	$n\sqrt{\frac{L}{\mu}}$	$\times \log\frac{1}{\varepsilon}$
SAG(A), SVRG, SDCA, MISO	$d\times$	$(n+\frac{L}{\mu})$	$\times \log\frac{1}{\varepsilon}$
Accelerated versions	$d\times$	$(n+\sqrt{n\frac{L}{\mu}})$	$\times \log\frac{1}{\varepsilon}$

- **Acceleration for special algorithms** (e.g., Shalev-Shwartz and Zhang, 2014; Nitanda, 2014; Lan, 2015; Defazio, 2016)

- **Catalyst** (Lin, Mairal, and Harchaoui, 2015a)
  - Widely applicable generic acceleration scheme

SGD minimizes the testing cost!

- **Goal**: minimize $f(\theta) = \mathbb{E}_{p(x,y)}\ell(y, h(x,\theta))$
  - Given n independent samples (x_i, y_i), $i = 1, \dots, n$ from $p(x,y)$
  - Given a single pass of stochastic gradient descent
  - Bounds on the excess testing cost $\mathbb{E}f(\bar{\theta}_n) - \inf_{\theta \in \mathbb{R}^d} f(\theta)$

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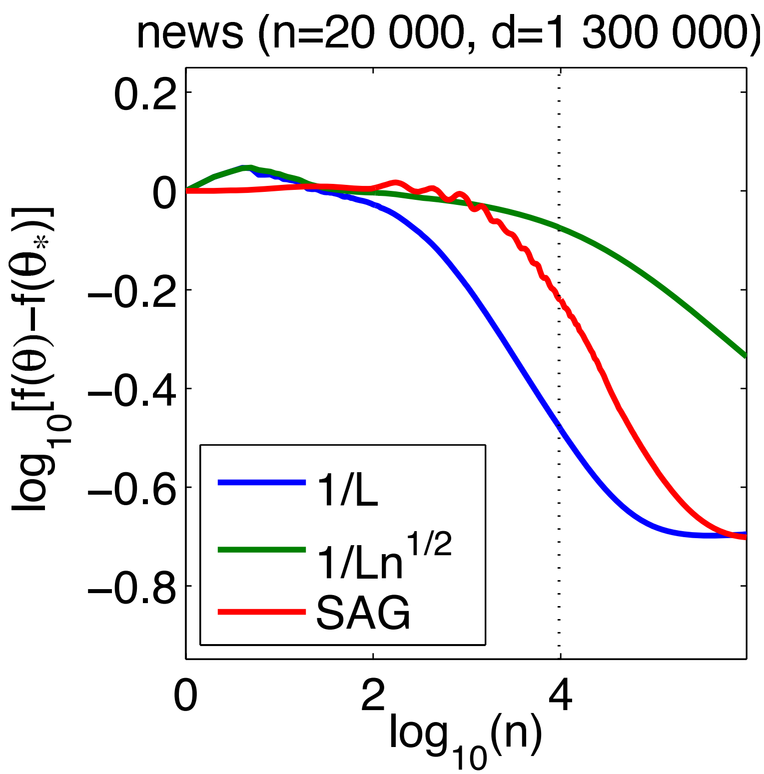
- **Constant-step-size SGD**
  - Linear convergence up to the noise level for strongly-convex problems (Solodov, 1998; Nedic and Bertsekas, 2000)
  - Full convergence and robustness to ill-conditioning?

Robust averaged stochastic gradient (Bach and Moulines, 2013)

- **Constant-step-size SGD is convergent for least-squares**
  - Convergence rate in $O(1/n)$ without any dependence on μ
  - Simple choice of step-size (equal to $1/L$) *(see board)*

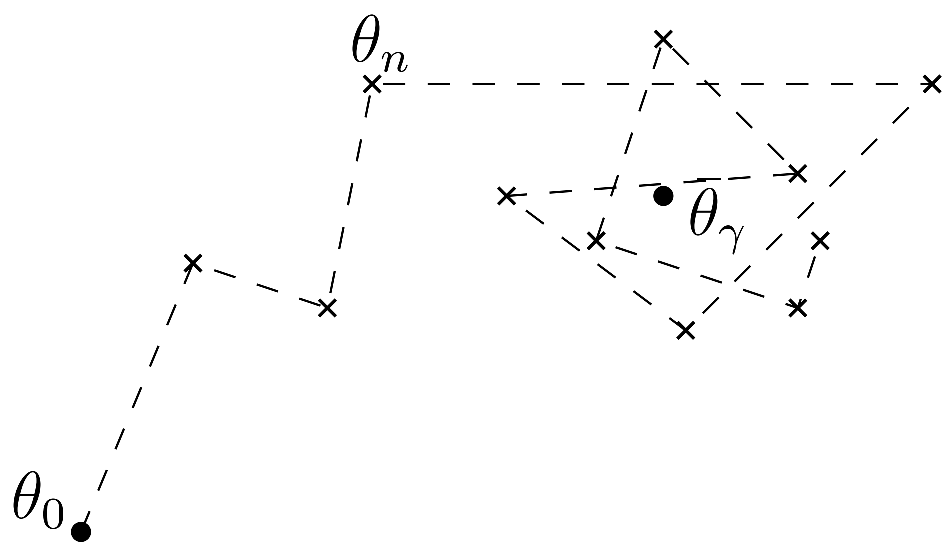


Markov chain interpretation of constant step sizes

- LMS recursion for $f_n(\theta) = \frac{1}{2}\big(y_n - \langle \Phi(x_n), \theta \rangle\big)^2$

$$\theta_n = \theta_{n-1} - \gamma\big(\langle \Phi(x_n), \theta_{n-1} \rangle - y_n\big)\Phi(x_n)$$

- The sequence $(\theta_n)_n$ is a homogeneous Markov chain
  - convergence to a stationary distribution π_γ
  - with expectation $\bar{\theta}_\gamma \stackrel{\text{def}}{=} \int \theta \pi_\gamma(\mathrm{d}\theta)$



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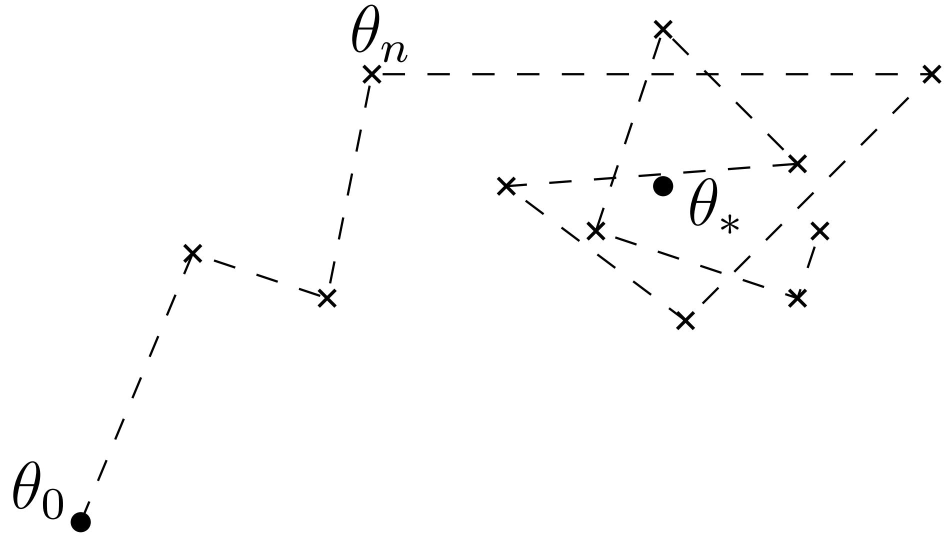

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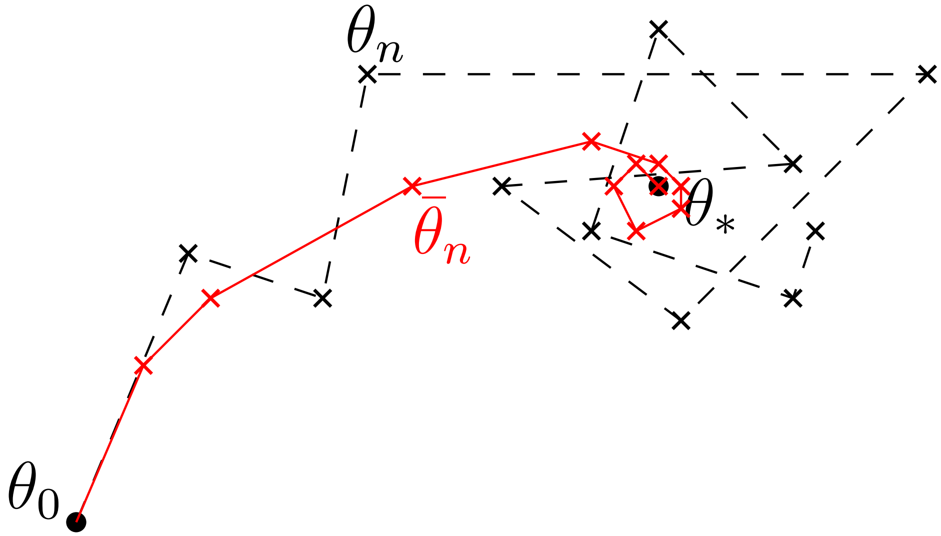

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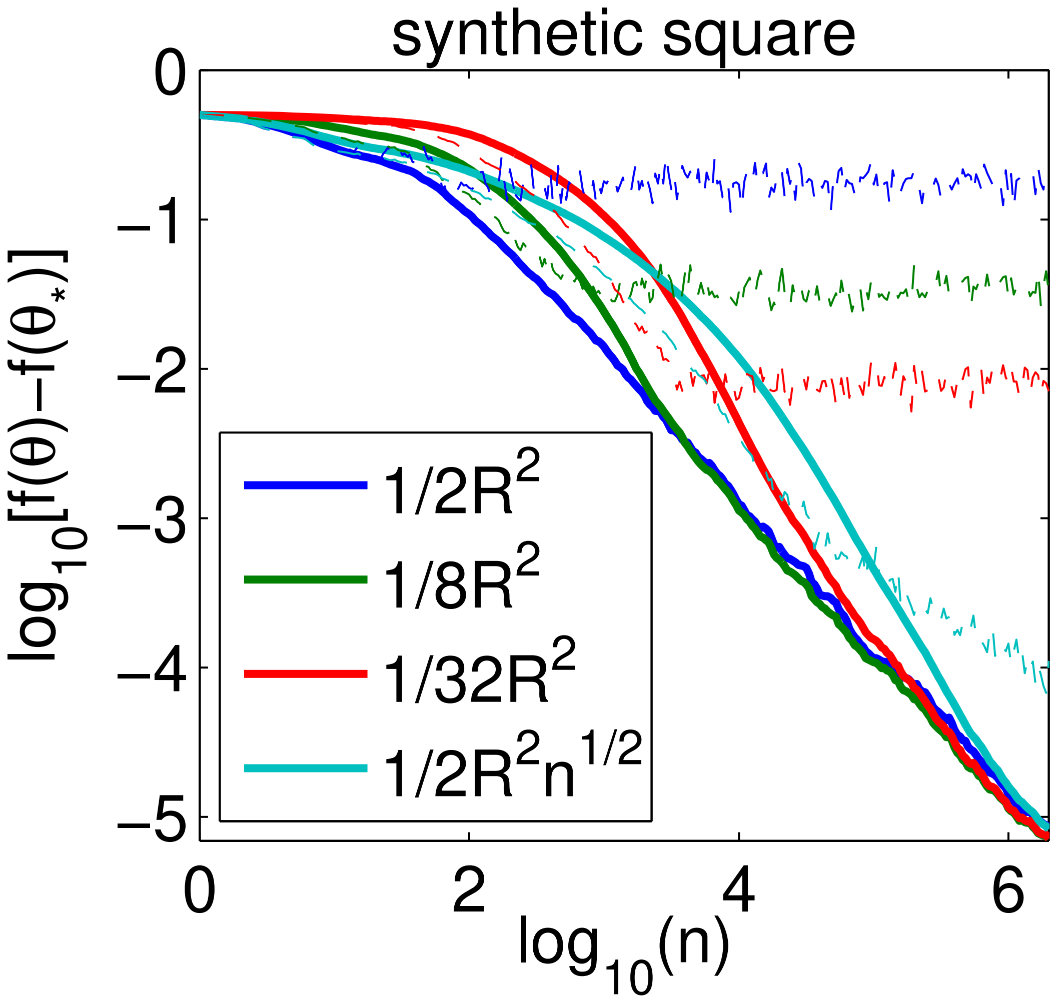
  - θ_n does not converge to θ_* but oscillates around it
  - oscillations of order $\sqrt{\gamma}$

- **Ergodic theorem:**
  - Averaged iterates converge to $\bar{\theta}_\gamma = \theta_*$ at rate $O(1/n)$

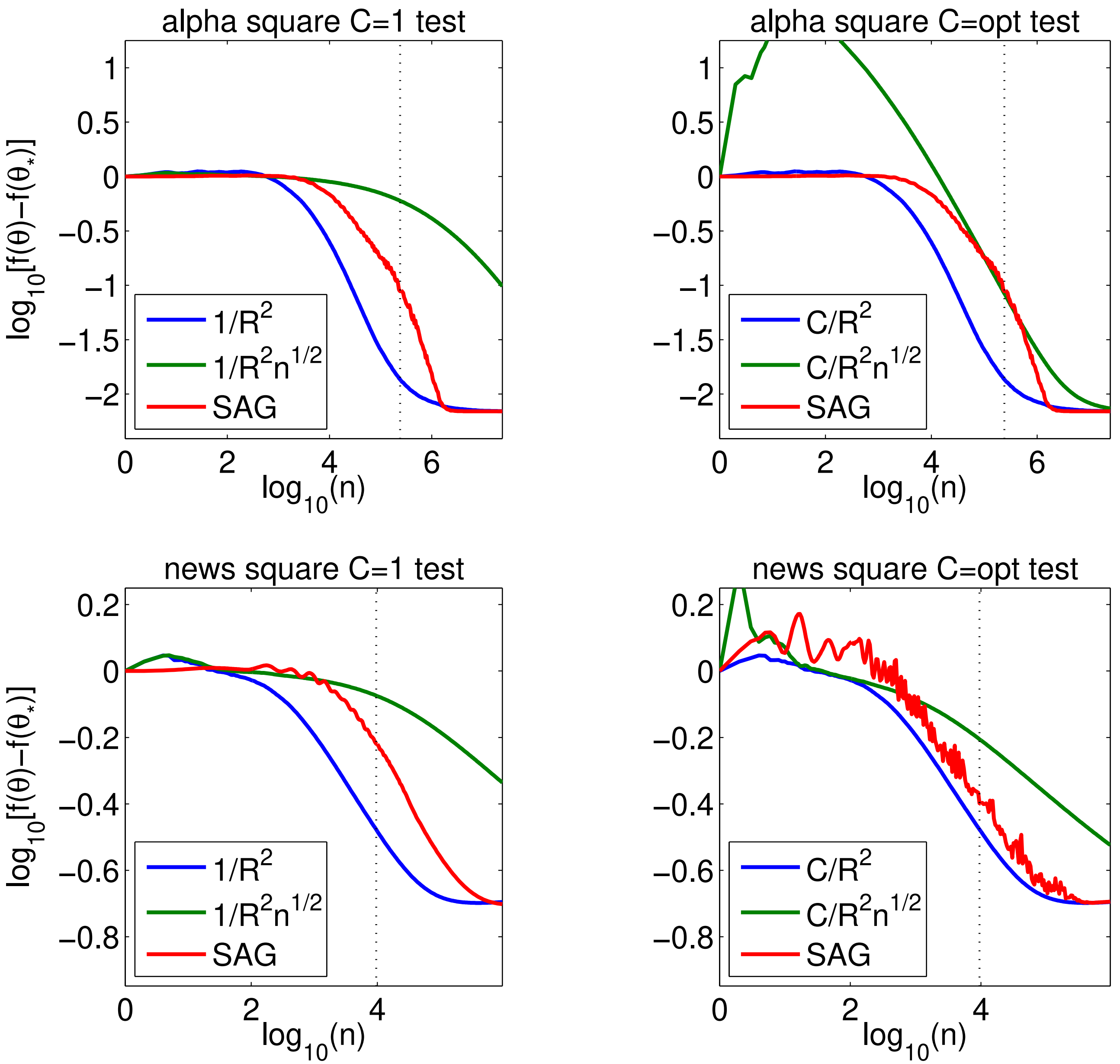
Simulations - synthetic examples

- Gaussian distributions - $p = 20$



Simulations - benchmarks

- *alpha* $(p = 500,\ n = 500\ 000)$, *news* $(p = 1\ 300\ 000,\ n = 20\ 000)$



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- **Multiple passes still work better in practice**
  - See Pillaud-Vivien, Rudi, and Bach (2018)

Perspectives

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  - Provable and precise rates
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  - Pre-conditioning

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
   - Constant step-sizes: for *testing* error

2. **Beyond convex problems**
   - Generic algorithms with generic “guarantees”
   - Global convergence for over-parameterized neural networks

Parametric supervised machine learning

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

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

data fitting term $+$ regularizer

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

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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)
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  - SVRG (Johnson and Zhang, 2013; Zhang et al., 2013)
  - MISO (Mairal, 2015), Finito (Defazio et al., 2014b)
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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 κ = condition number)

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

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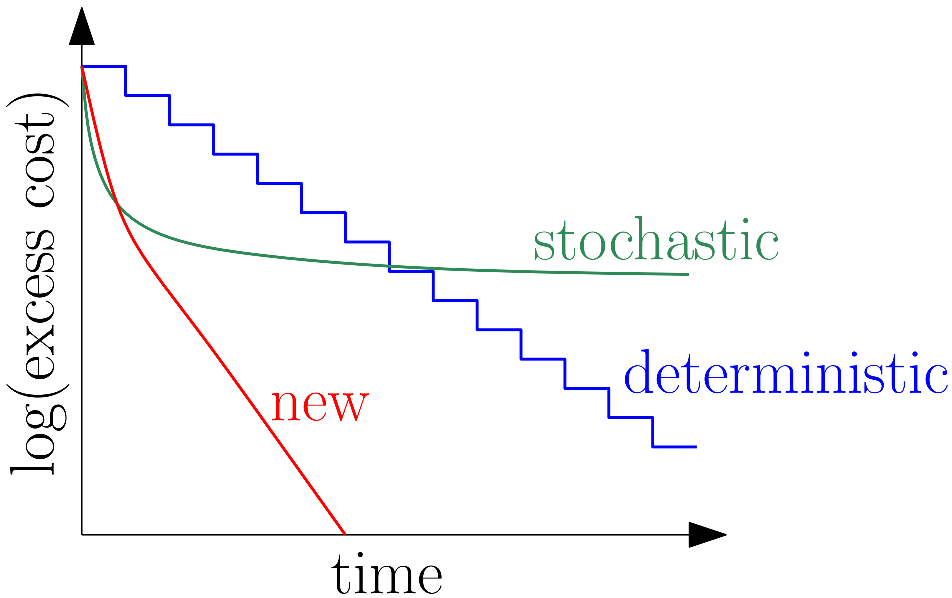
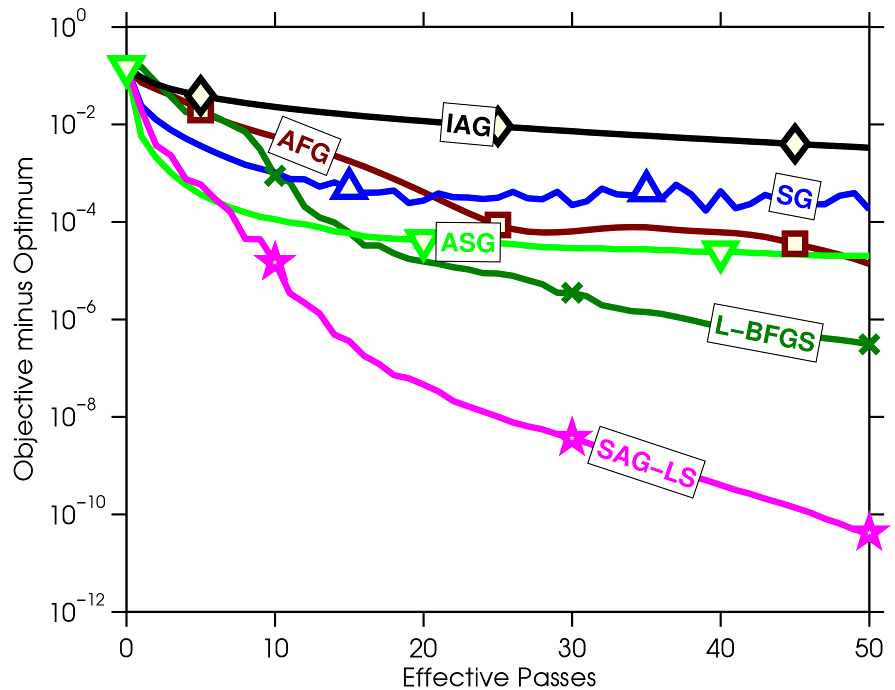
- **Matching lower bounds** (Woodworth and Srebro, 2016; Lan, 2015)

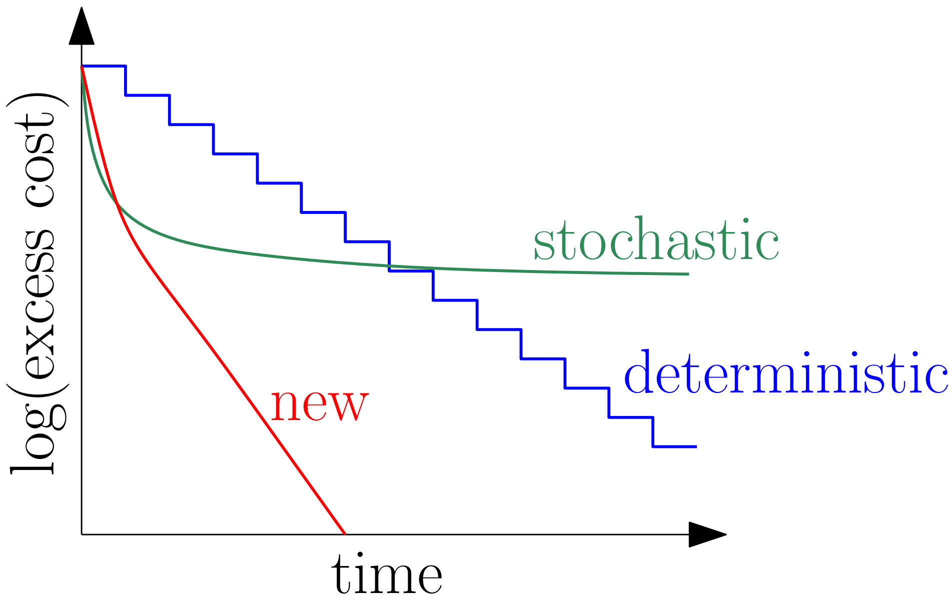
Exponentially convergent SGD for finite sums
From theory to practice and vice-versa

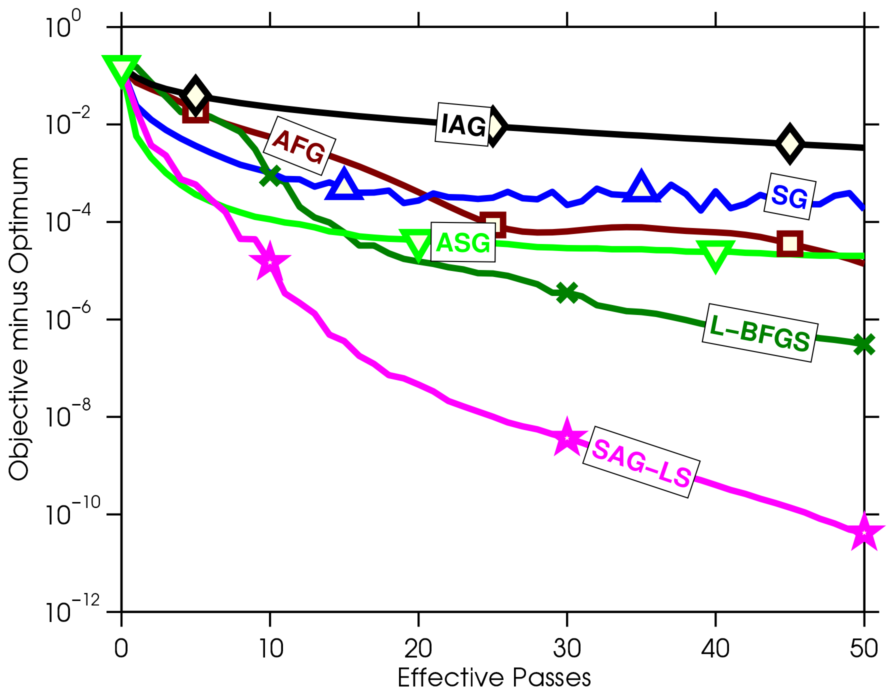




- **Empirical performance "matches" theoretical guarantees**

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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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
  - From least-squares to convex losses
  - High-dimensional inference
  - Non-parametric regression
  - Randomized linear algebra
  - Bandit problems
  - etc...

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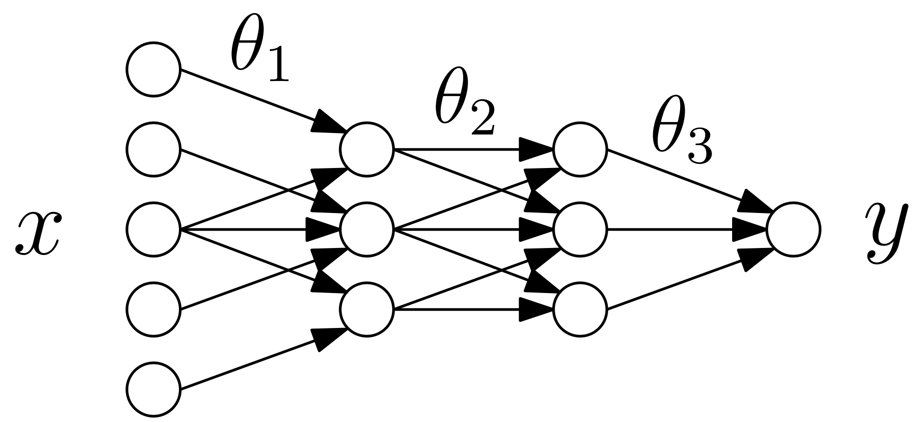
- **What about deep learning?**

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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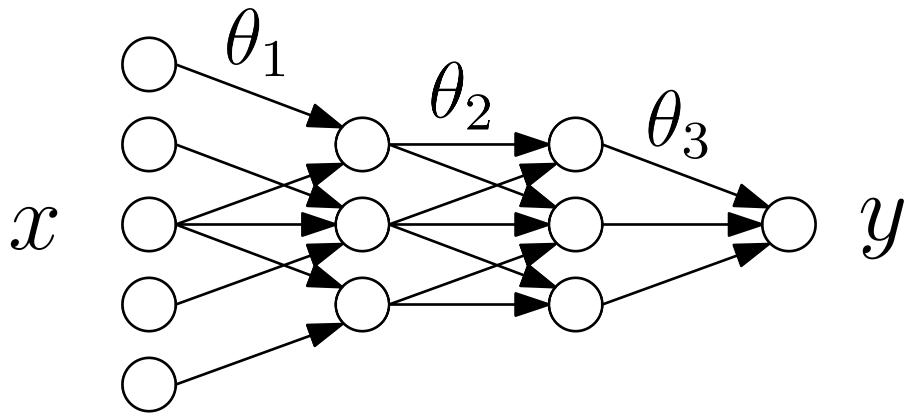

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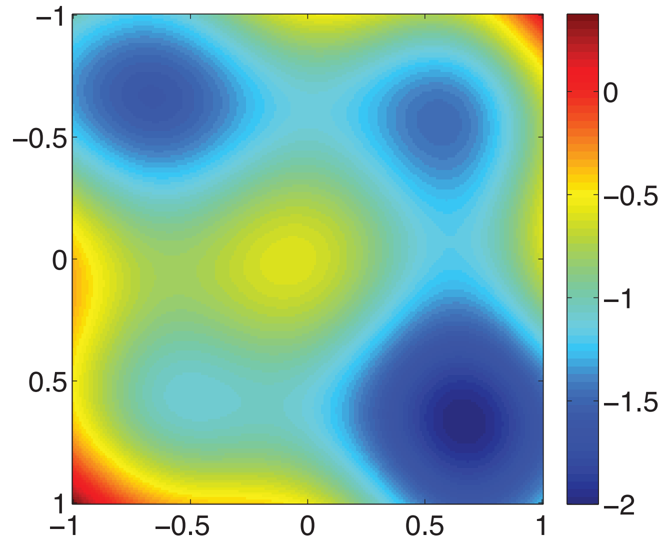
- **Main difficulties**

  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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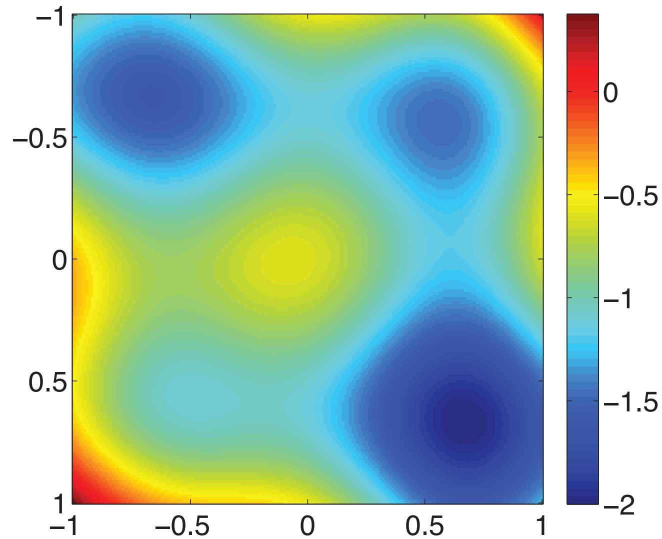

  - Local minima
  - Stationary points
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- **Generic local theoretical guarantees**
  - Convergence to stationary points or local minima
  - See, e.g., Lee et al. (2016); Jin et al. (2017)

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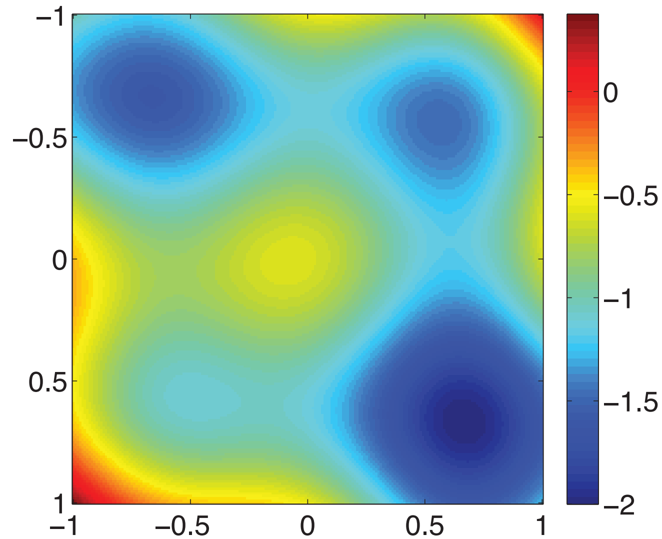

- **General global performance guarantees impossible to obtain**

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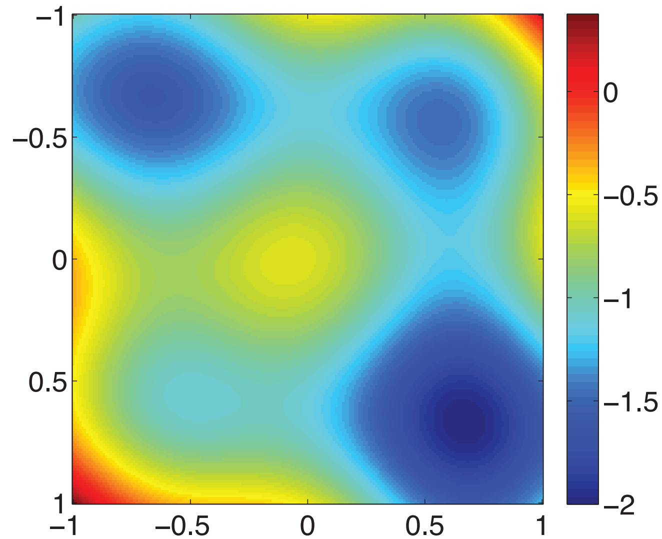

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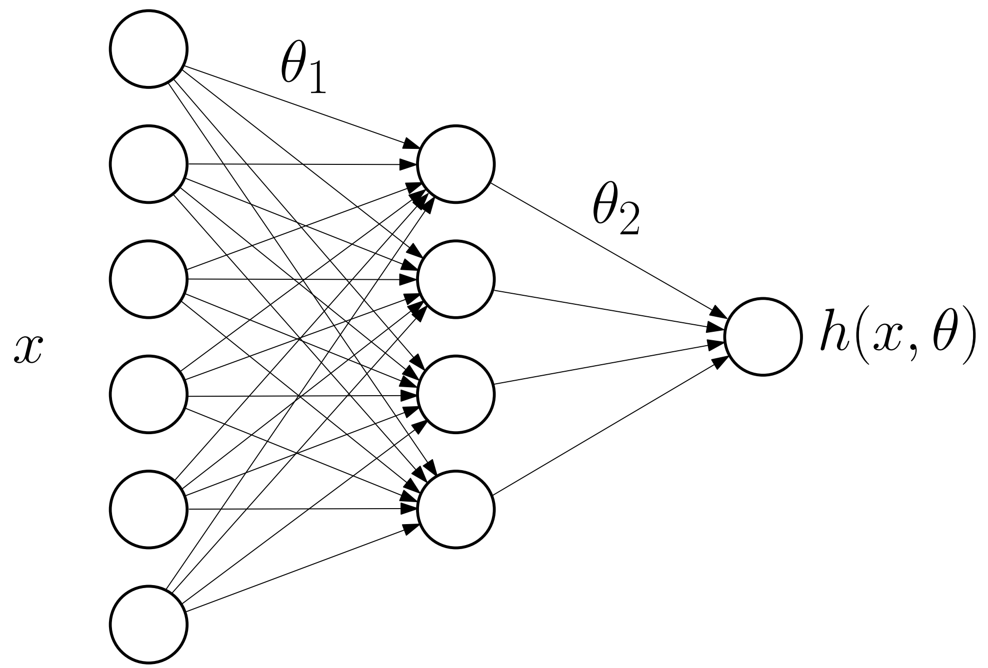
- **Special case of (deep) neural networks**
  - Most local minima are equivalent (Choromanska et al., 2015)
  - No spurrious local minima (Soltanolkotabi et al., 2018)

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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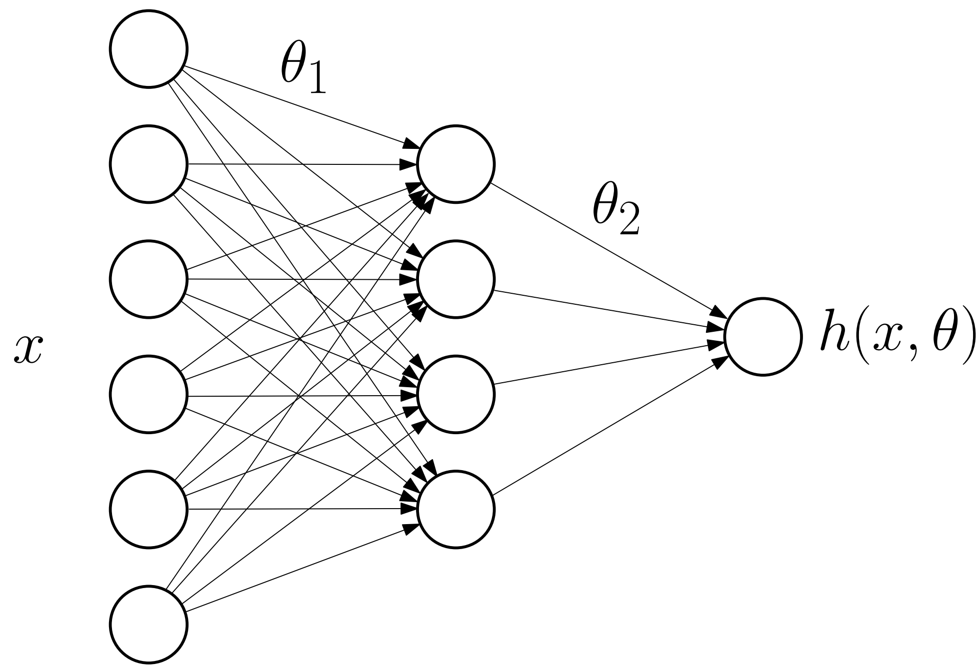

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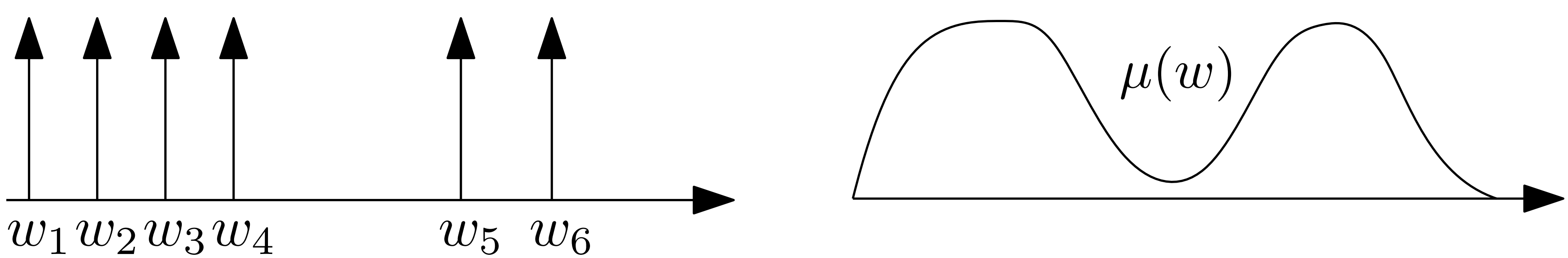
  - $h = \dfrac{1}{m}\displaystyle\sum_{j=1}^m \Psi(w_j) = \int_{\mathcal{W}} \Psi(w)d\mu(w)$ with $d\mu(w) = \dfrac{1}{m}\displaystyle\sum_{j=1}^m \delta_{w_j}$



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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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- **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 (see Chizat and Bach, 2020)

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

- **General framework**: minimize $F(\mu) = R\Big(\int_{\mathcal{W}} \Psi(w) d\mu(w) \Big)$
  - 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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  - 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, 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)

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  - Applies to rectified linear units (but also to sigmoid activations)

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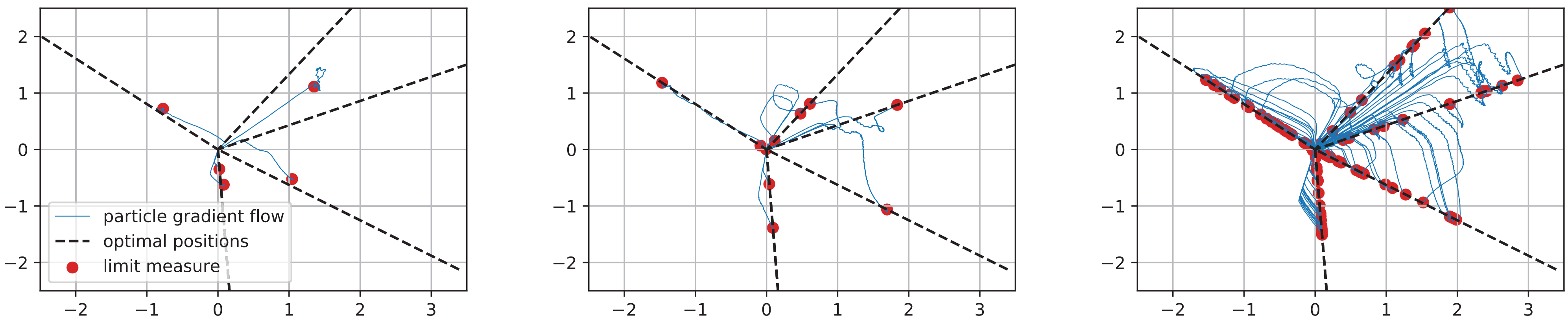
- **Only qualititative!**

Simple simulations with neural networks

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



5 neurons 10 neurons 100 neurons

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

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

NB : also applies to spike deconvolution

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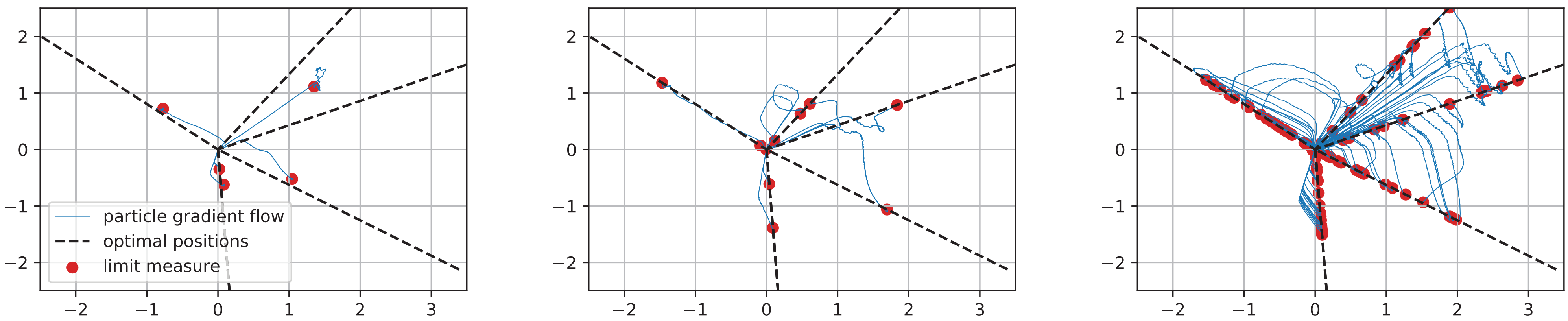

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From qualitative to quantitative results ?

- **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 bursty activity on ArXiv**
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- **Any link?**

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- **Equivalence to "lazy" training** (Chizat and Bach, 2018b)
  - Convergence to a positive-definite kernel method
  - Neurons move infinitesimally
  - Extension of results from Jacot et al. (2018)

Lazy training (Chizat and Bach, 2018b)

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

- **Consequence**: around $W(0)$, $G_\alpha(W)$ has
  - Gradient "proportional" to $\nabla R(\alpha h(W(0)))/\alpha$
  - Hessian "proportional" to $\nabla^2 R(\alpha h(W(0)))$

Lazy training (Chizat and Bach, 2018b)

- **Generic criterion $G(W) = R(h(W))$ to minimize w.r.t. W**
  - Example: R loss, $h(W) = \frac{1}{m}\sum_{i=1}^{m} \Psi(w_i)$ prediction function
  - Introduce (large) scale factor $\alpha > 0$ and $G_\alpha(W) = R(\alpha h(W))/\alpha^2$
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- **Proposition** (informal, see paper for precise statement)
  - Assume differential of h at $W(0)$ is surjective
  - Gradient flow $\dot{W} = -\nabla G_\alpha(W)$ is such that

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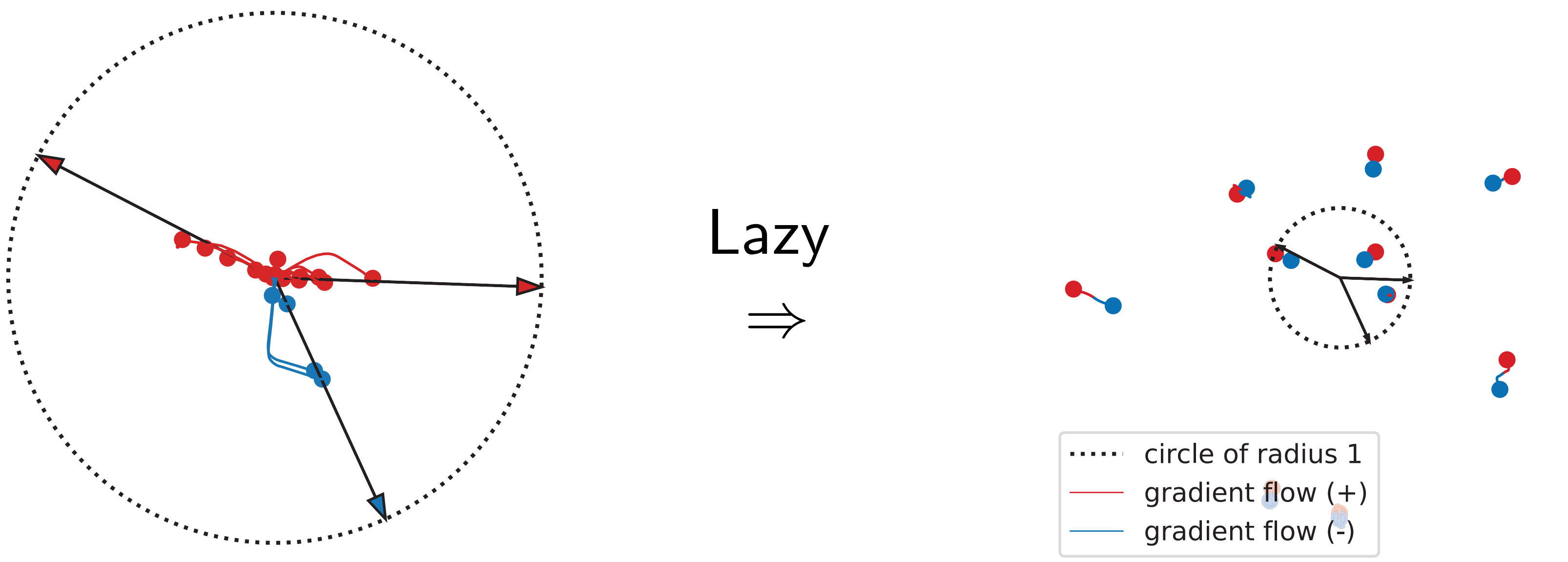

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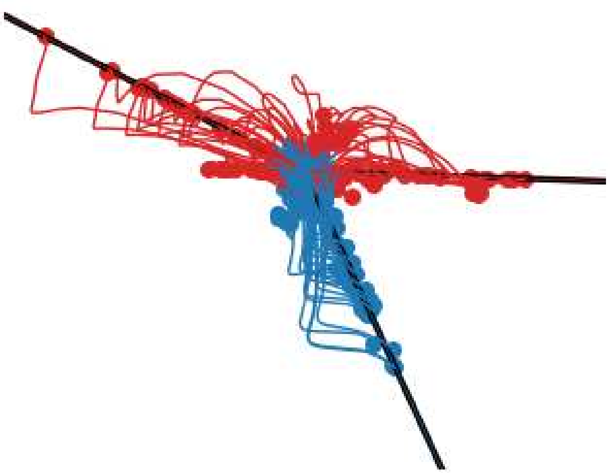

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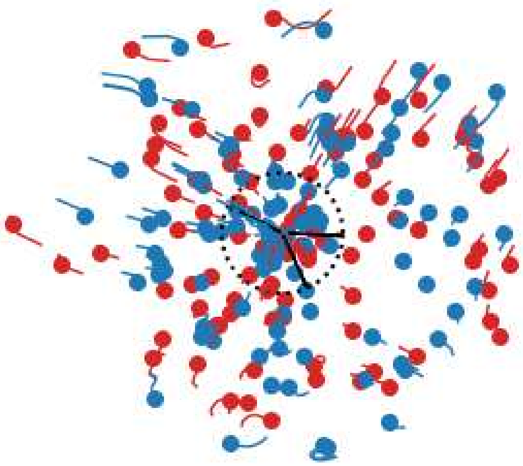
$\Rightarrow$



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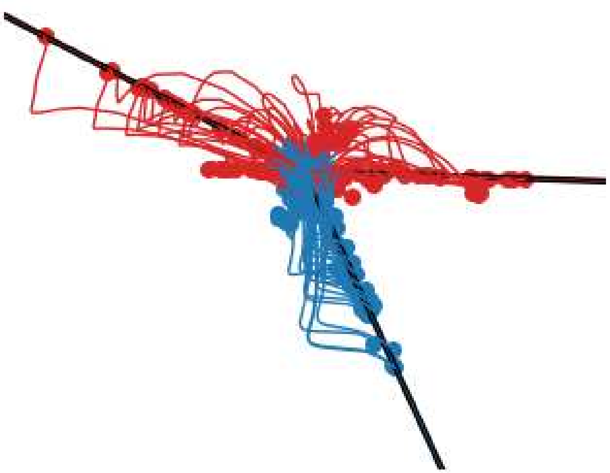

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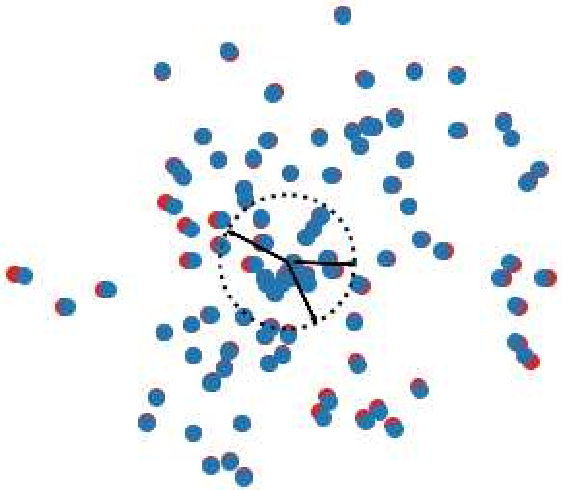

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$\Rightarrow$ Equivalent to a linear model
$h(W) \approx h(W(0)) + (W - W(0))^\top \nabla h(W(0))$

From lazy training to neural tangent kernel

- **Neural tangent kernel** (Jacot et al., 2018; Lee et al., 2019)
  - Linear model: $h(x, W) \approx h(x, W(0)) + (W - W(0))^\top \nabla h(x, W(0))$
  - Corresponding kernel $k(x, x') = \nabla h(x, W(0))^\top \nabla h(x', W(0))$
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- **Two questions**:
  - Does this really "demystify" generalization in deep networks?
    (are state-of-the-art neural networks in the lazy regime?)
  - Can kernel methods beat neural networks?
    (is the neural tangent kernel useful in practice?)

Are state-of-the-art neural networks in the lazy regime?

- **Lazy regime**: Neurons move infinitesimally

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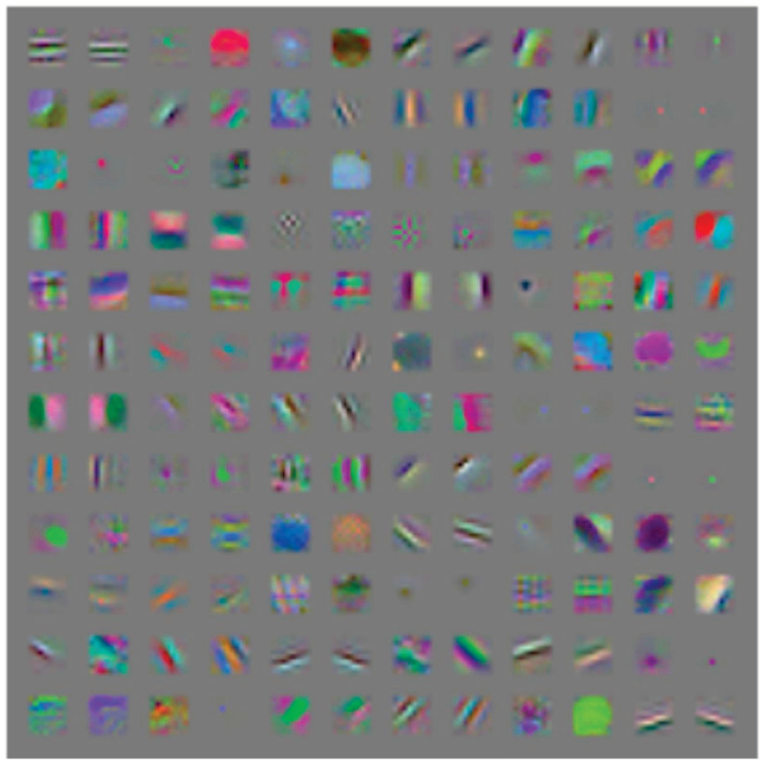

From Goodfellow, Bengio, and Courville (2016)

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- **Lazy regime**: Neurons move infinitesimally
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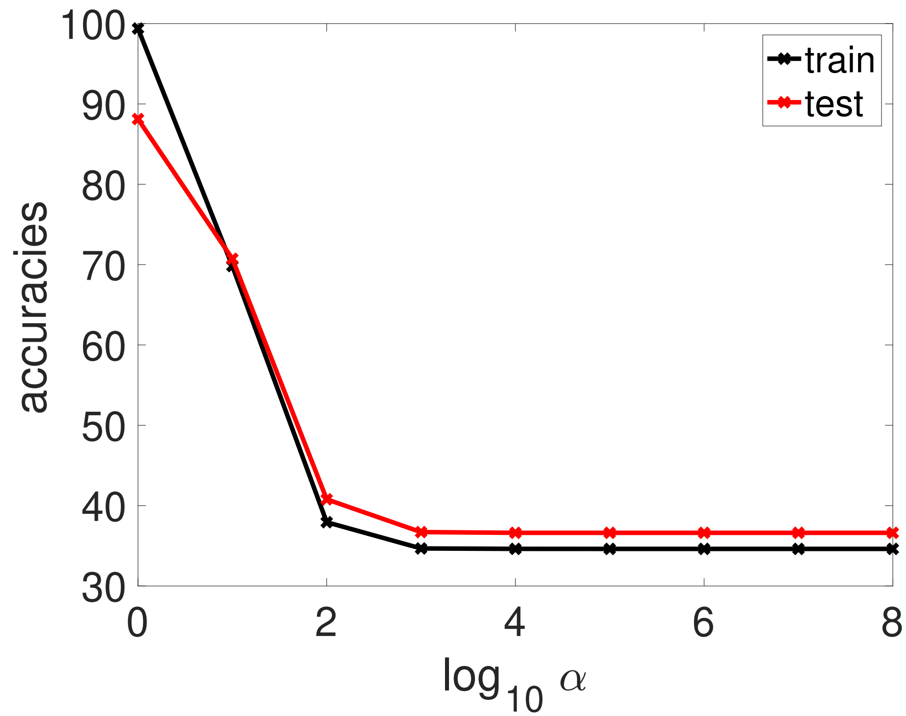
- **Evidence 3**: Take a state-of-the-art CNN and make it lazier
  - Chizat, Oyallon, and Bach (2019)

Lazy training seen in practice?

- **Convolutional neural network**
  - “VGG-11”: 10 millions parameters
  - “CIFAR10” images: 60 000 32×32 color images and 10 classes
  - (almost) state-of-the-art accuracies



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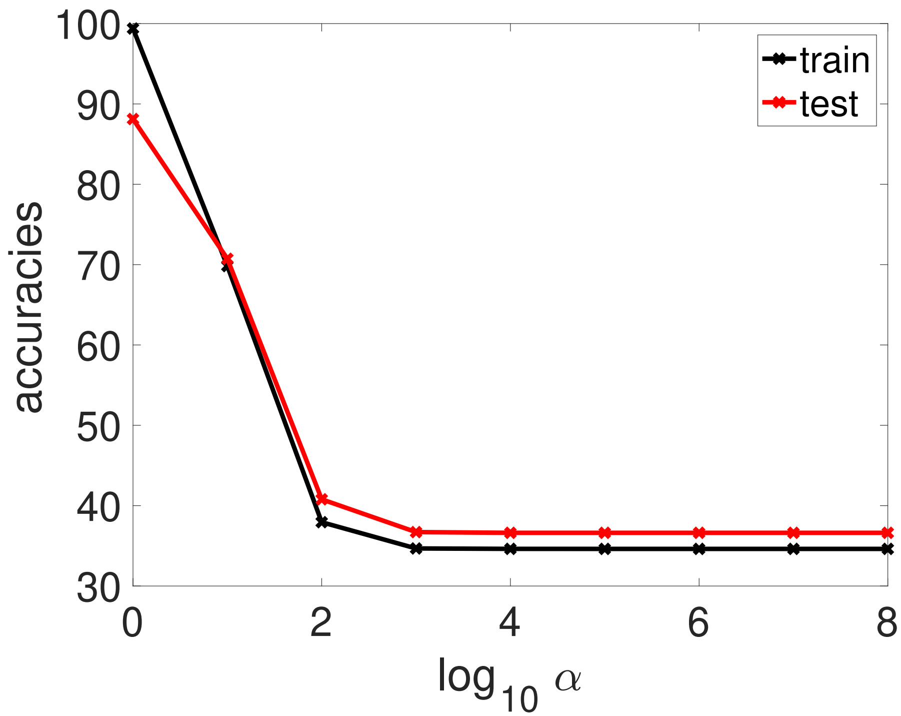

- **Understanding the mix of lazy and non-lazy regimes?**

Is the neural tangent kernel useful in practice?

- **Fully connected networks**
  - Gradient with respect to output weights: classical random features (Rahimi and Recht, 2007)
  - Gradient with respect to input weights: extra random features
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- **Convolutional neural networks**
  - Theoretical and computational properties (Arora et al., 2019)
  - Good stability properties (Bietti and Mairal, 2019)
  - Can achieve state-of-the-art performance with additional tricks (Mairal, 2016; Novak et al., 2018) on the CIFAR10 dataset (Li et al., 2019)

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- **Going further without explicit representation learning?**

Healthy interactions between theory, applications, and hype?

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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.

Conclusions
Optimization for machine learning

- **Well understood**
  - Convex case with a single machine
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  - Non-convex case: SGD for local risk minimization

- **Not well understood**: many open problems
  - Step-size schedules and acceleration
  - Dealing with non-convexity
    (global minima vs. local minima and stationary points)
  - Distributed learning: multiple cores, GPUs, and cloud (see, e.g., Hendrikx, Bach, and Massoulié, 2019, and references therein)

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