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

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  Big data $\rightarrow$ Data science $\rightarrow$ Machine Learning
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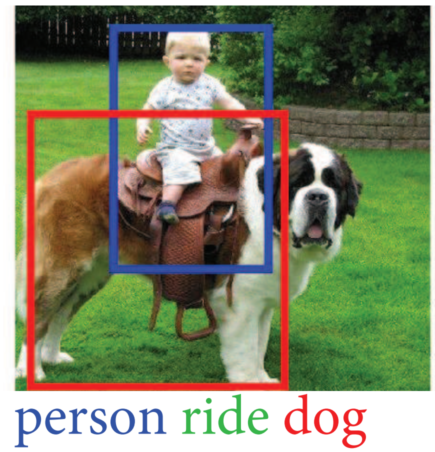
- **Healthy interactions between theory, applications, and hype?**

Recent progress in perception (vision, audio, text)

From translate.google.fr



From Peyré et al. (2017)

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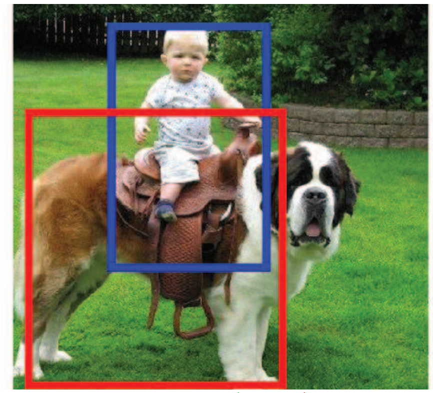

person ride dog

From Peyré et al. (2017)

(1) **Massive data**

(2) **Computing power**

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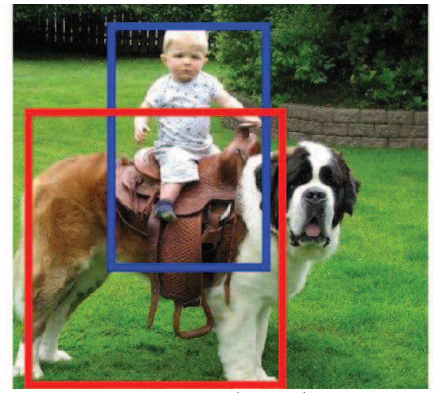

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+ computing power

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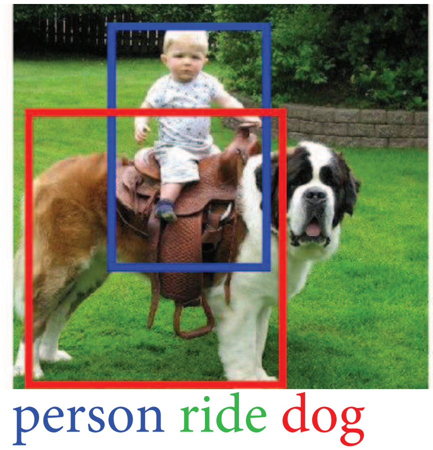

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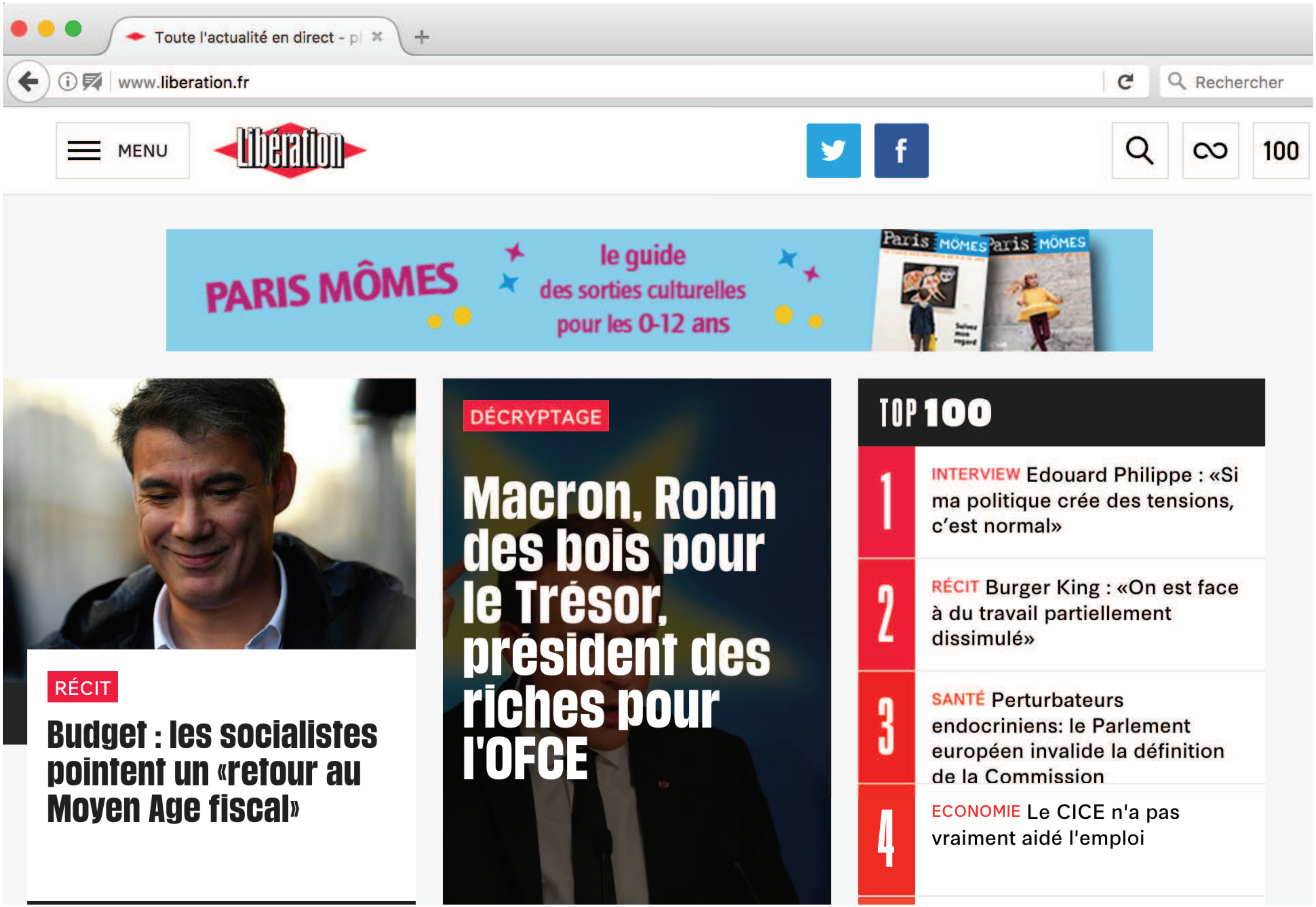
Machine learning for large-scale data

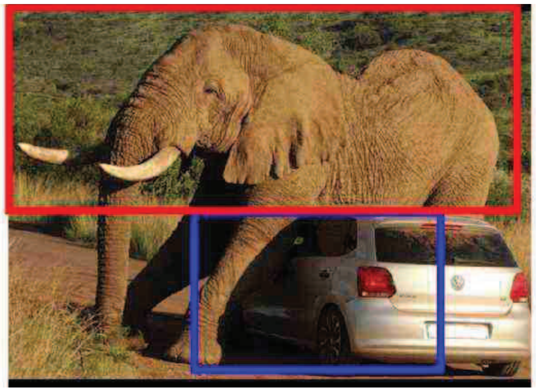
- **Large-scale supervised machine learning**: **large d, large n**
  - d : dimension of each observation (input) or number of parameters
  - n : number of observations

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

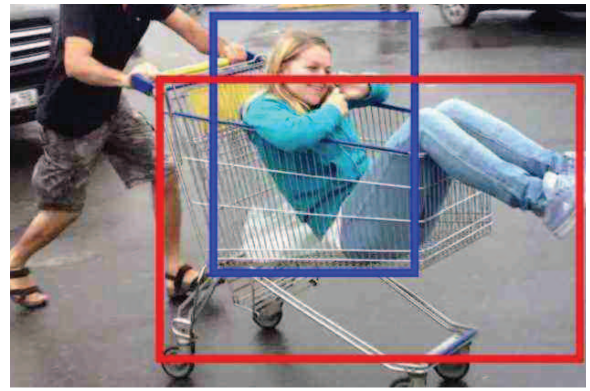
Advertising



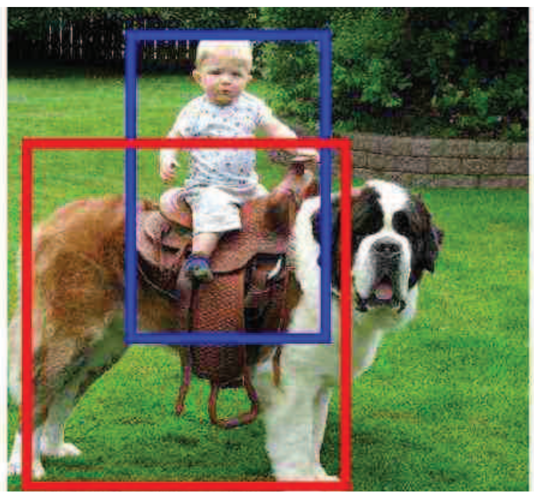
Object / action recognition in images



car under elephant



person in cart

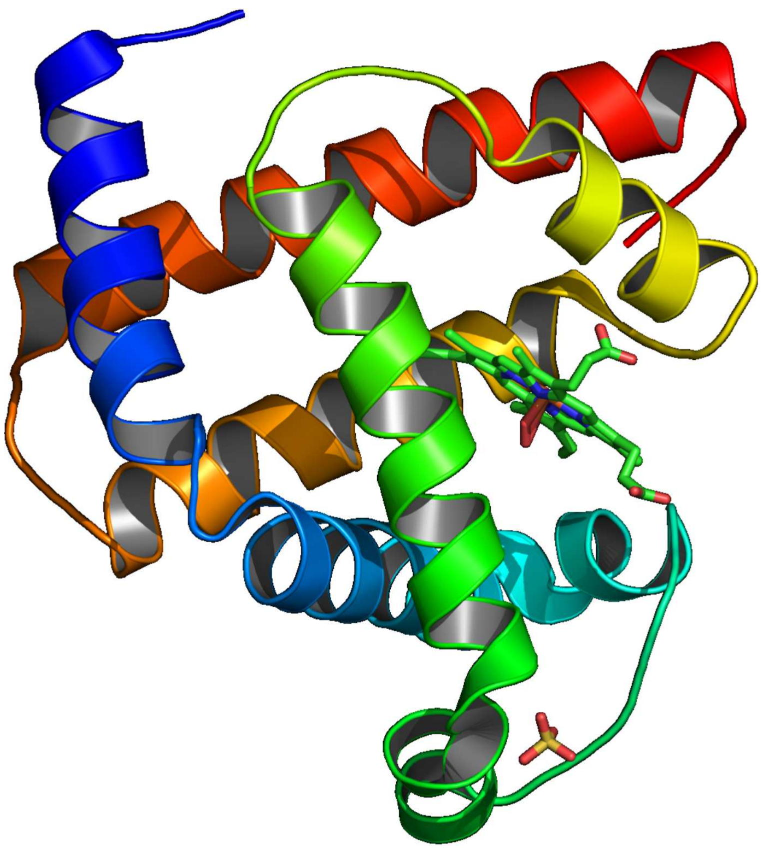


person ride dog

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**: $O(dn)$

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

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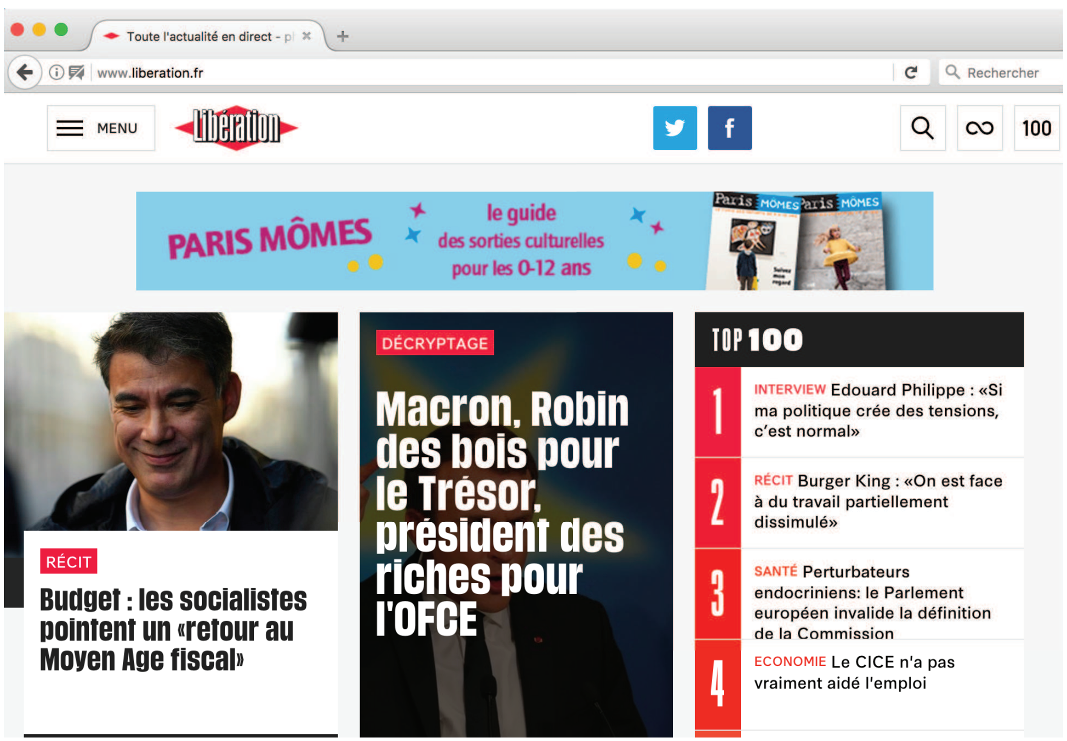

- **Advertising**: $n > 10^9$
  - $\Phi(x) \in \{0, 1\}^d$, $d > 10^9$
  - Navigation history + ad

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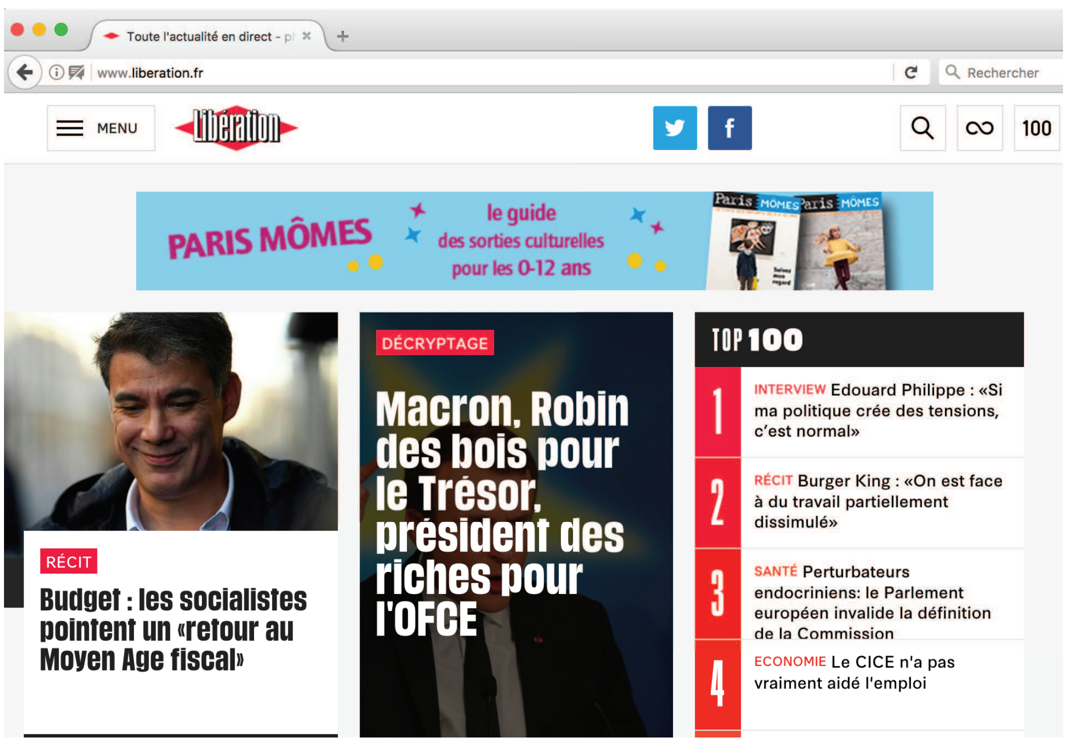

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- Linear predictions
  - $h(x, \theta) = \theta^\top \Phi(x)$

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x_1 x_2 x_3 x_4 x_5 x_6

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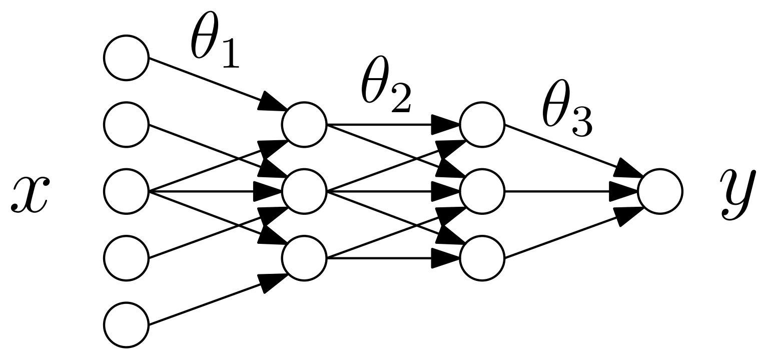
  - Neural networks ($n, d > 10^6$): $h(x, \theta) = \theta_m^\top \sigma(\theta_{m-1}^\top \sigma(\cdots \theta_2^\top \sigma(\theta_1^\top x))$



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

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

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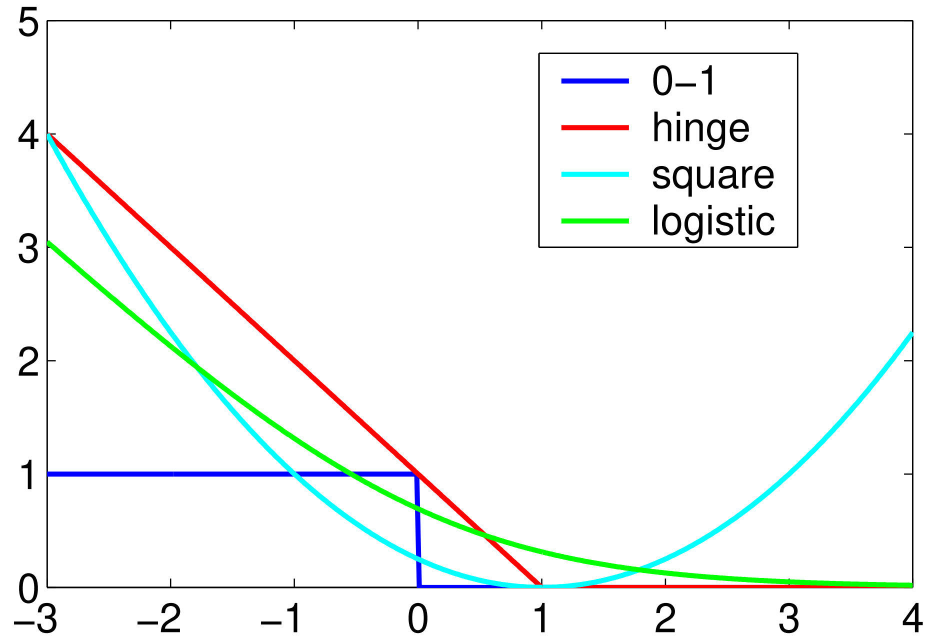
- **Classification** : $y \in \{-1,1\}$, prediction $\hat{y} = \text{sign}(h(x,\theta))$
  - loss of the form $\ell(y\,h(x,\theta))$
  - "True" 0-1 loss: $\ell(y\,h(x,\theta)) = 1_{y\,h(x,\theta)<0}$
  - Usual convex losses:



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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- 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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data fitting term $+$ regularizer

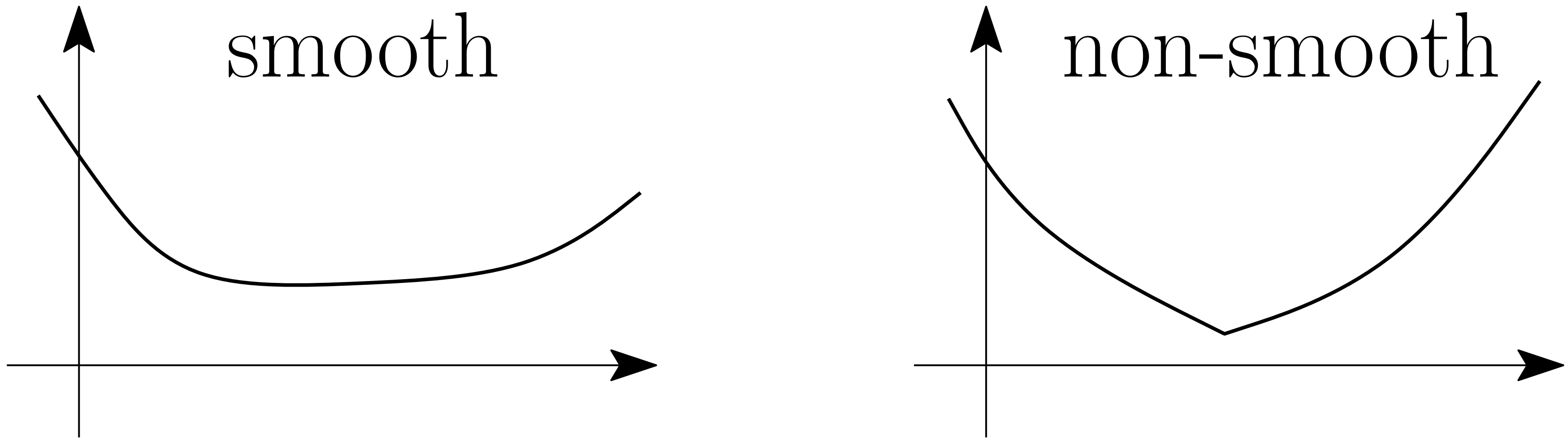
- Optimization: optimization of regularized risk training cost

- 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

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



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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

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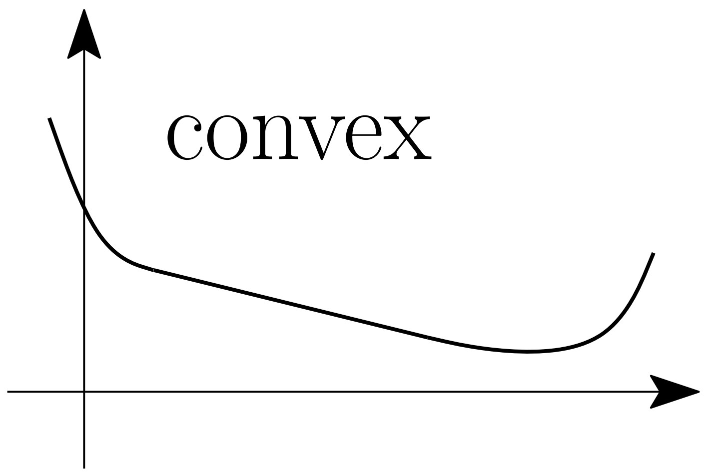
- Hessian $g''(\theta) = \dfrac{1}{n}\displaystyle\sum_{i=1}^{n} \ell''(y_i, \theta^\top \Phi(x_i))\Phi(x_i)\Phi(x_i)^\top$
  - Smooth loss $\Rightarrow \ell''(y_i, \theta^\top \Phi(x_i))$ bounded

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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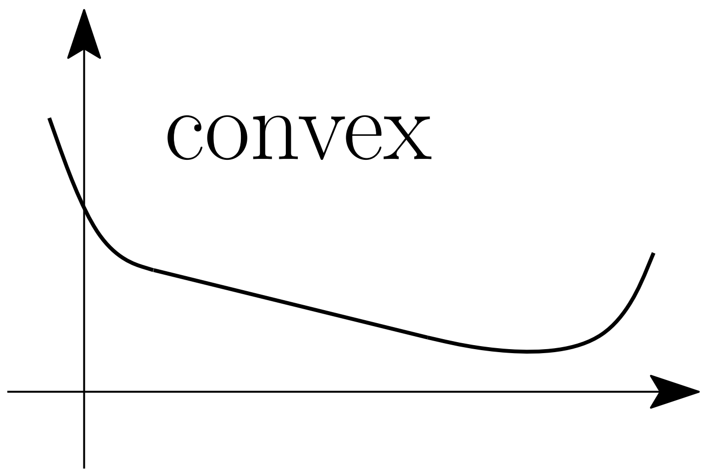

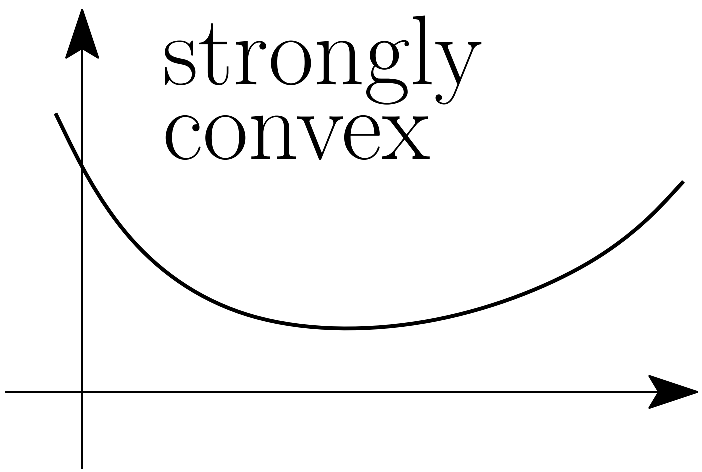

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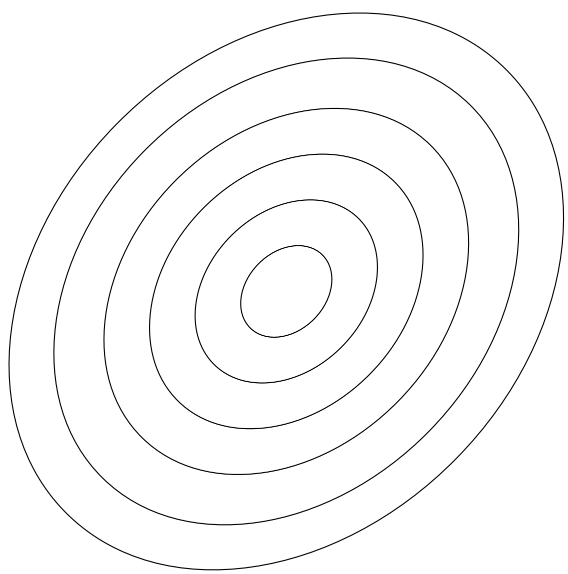
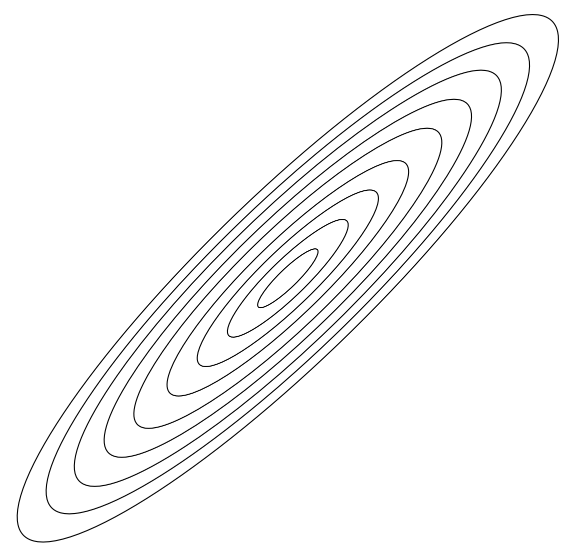
  – Condition number $\kappa = L/\mu \geqslant 1$



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

Board

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- Hessian $g''(\theta) = \dfrac{1}{n}\displaystyle\sum_{i=1}^{n} \ell''(y_i, \theta^\top \Phi(x_i))\Phi(x_i)\Phi(x_i)^\top$
  - 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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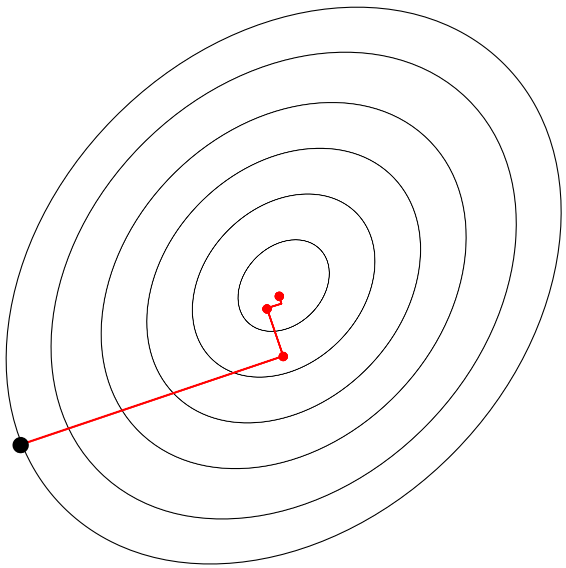
  - Even when $\mu > 0$, μ may be arbitrarily small!

- **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)*



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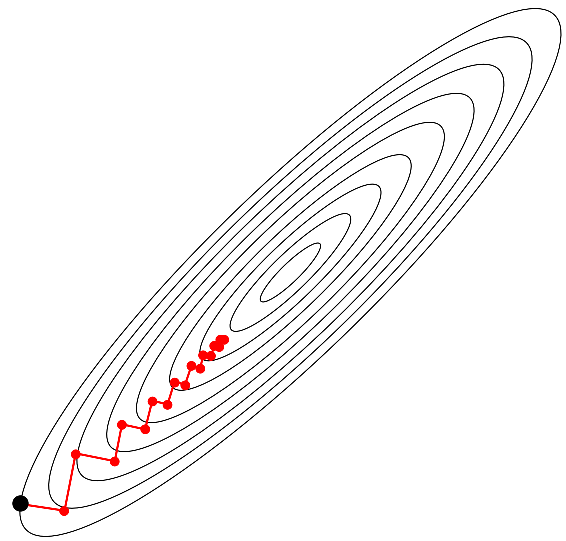

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Iterative methods for minimizing smooth functions

- **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)*

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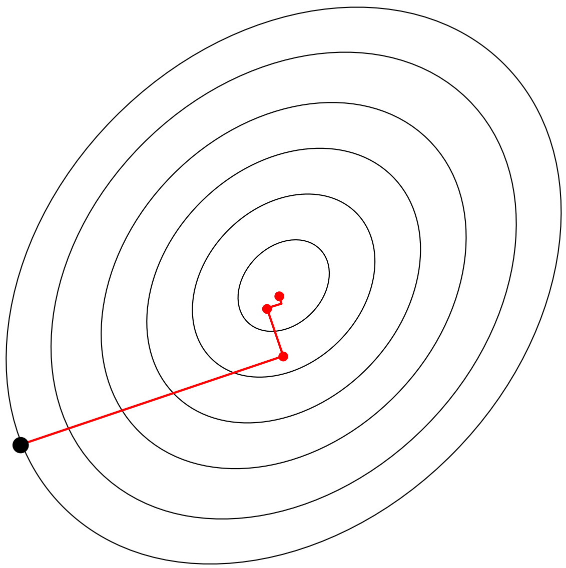

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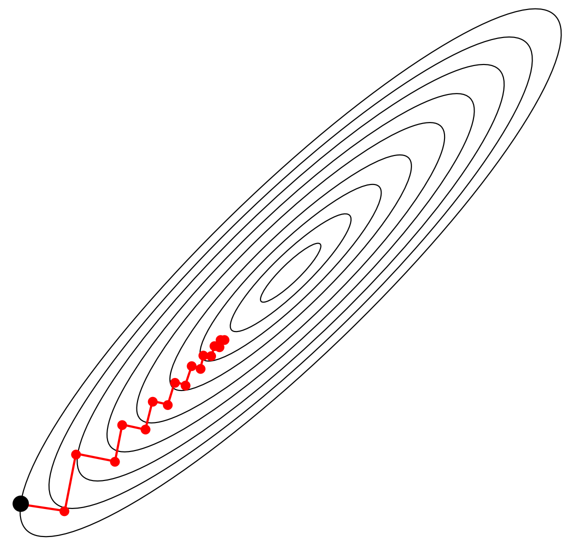

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Gradient descent - Proof for quadratic functions

- 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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- **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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\end{aligned}$$

- **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: $\|\theta_t - \theta_*\|^2 \leqslant \|\theta_0 - \theta_*\|^2$

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

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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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- **Key insights for machine learning (Bottou and Bousquet, 2008)**
  1. No need to optimize below statistical error
  2. Cost functions are averages
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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
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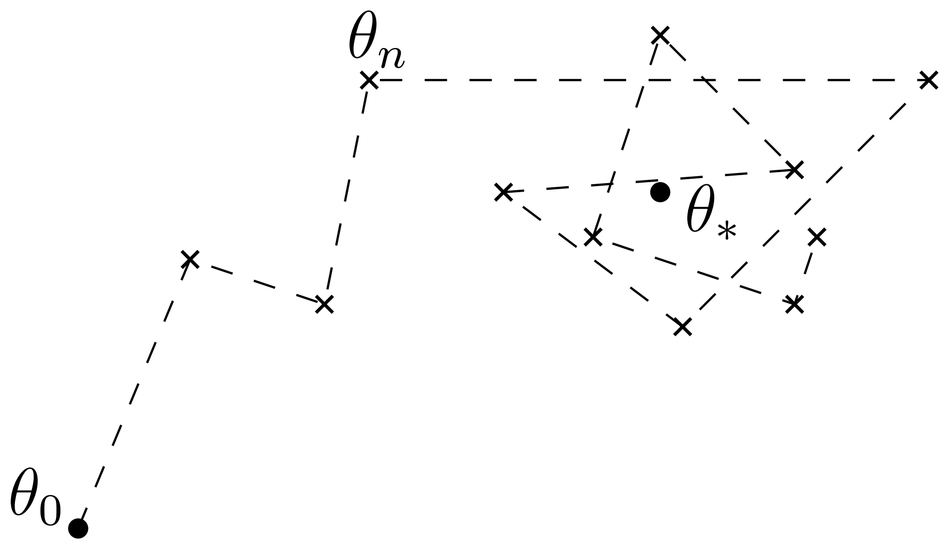
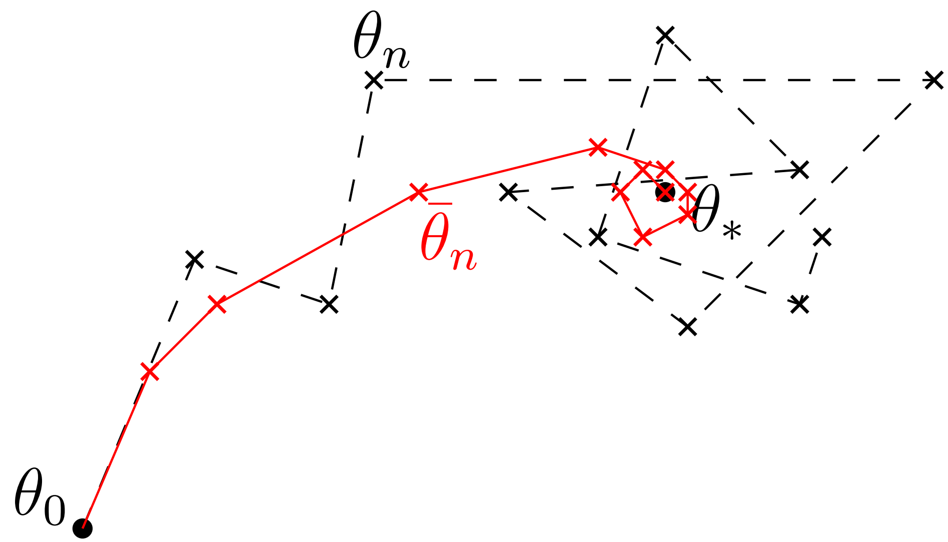
  - Robustness to the choice of C
- **Convergence rates** for $\mathbb{E}\|\theta_t - \theta_*\|^2$ and $\mathbb{E}\|\bar{\theta}_t - \theta_*\|^2$
  - no averaging: $O\Big(\frac{\sigma^2\gamma_t}{\mu}\Big) + O(e^{-\mu t \gamma_t})\|\theta_0 - \theta_*\|^2$
  - averaging: $\frac{\operatorname{tr} H(\theta_*)^{-1}}{t} + O\Big(\frac{\|\theta_0 - \theta_*\|^2}{\mu^2 t^2}\Big)$

    (see board)

Board

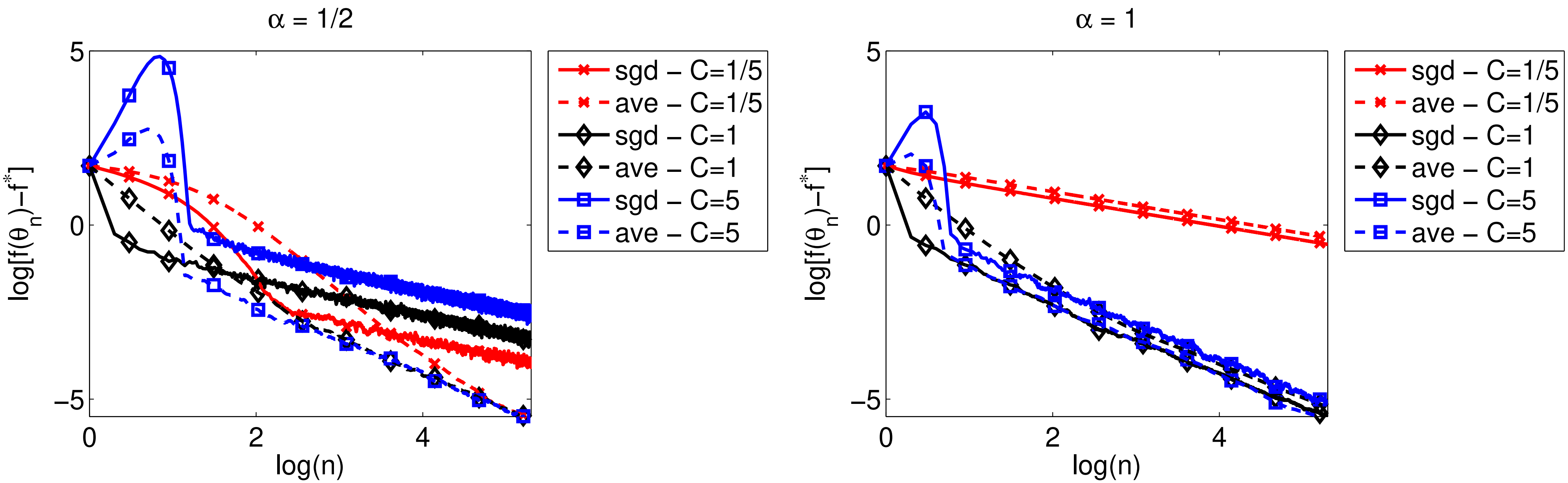
- Leaving initial point θ_0 to reach θ_*
- Impact of averaging





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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  - Iteration complexity is linear in n

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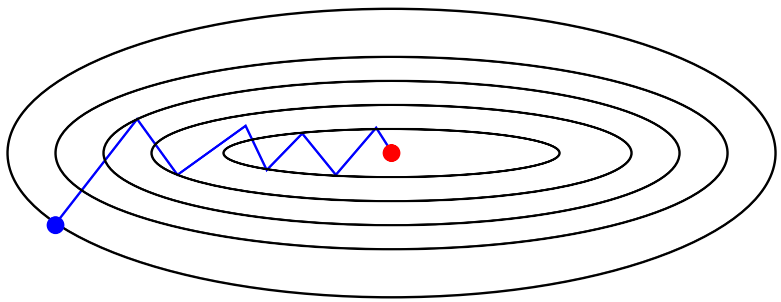

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  - Iteration complexity is independent of n

Stochastic vs. deterministic methods

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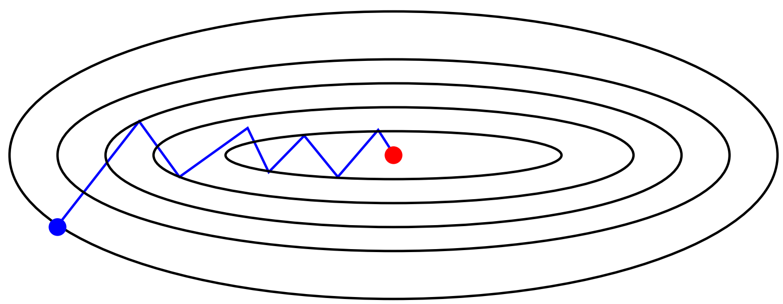

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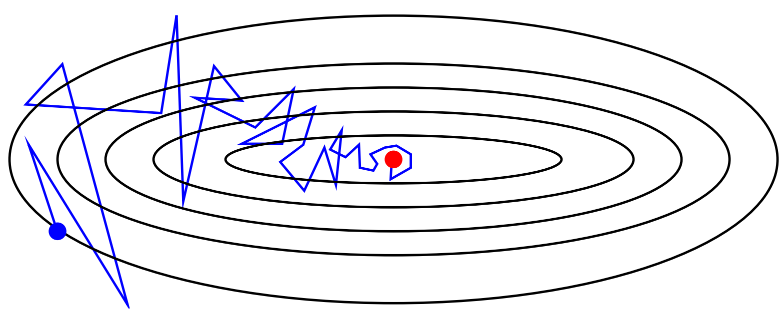
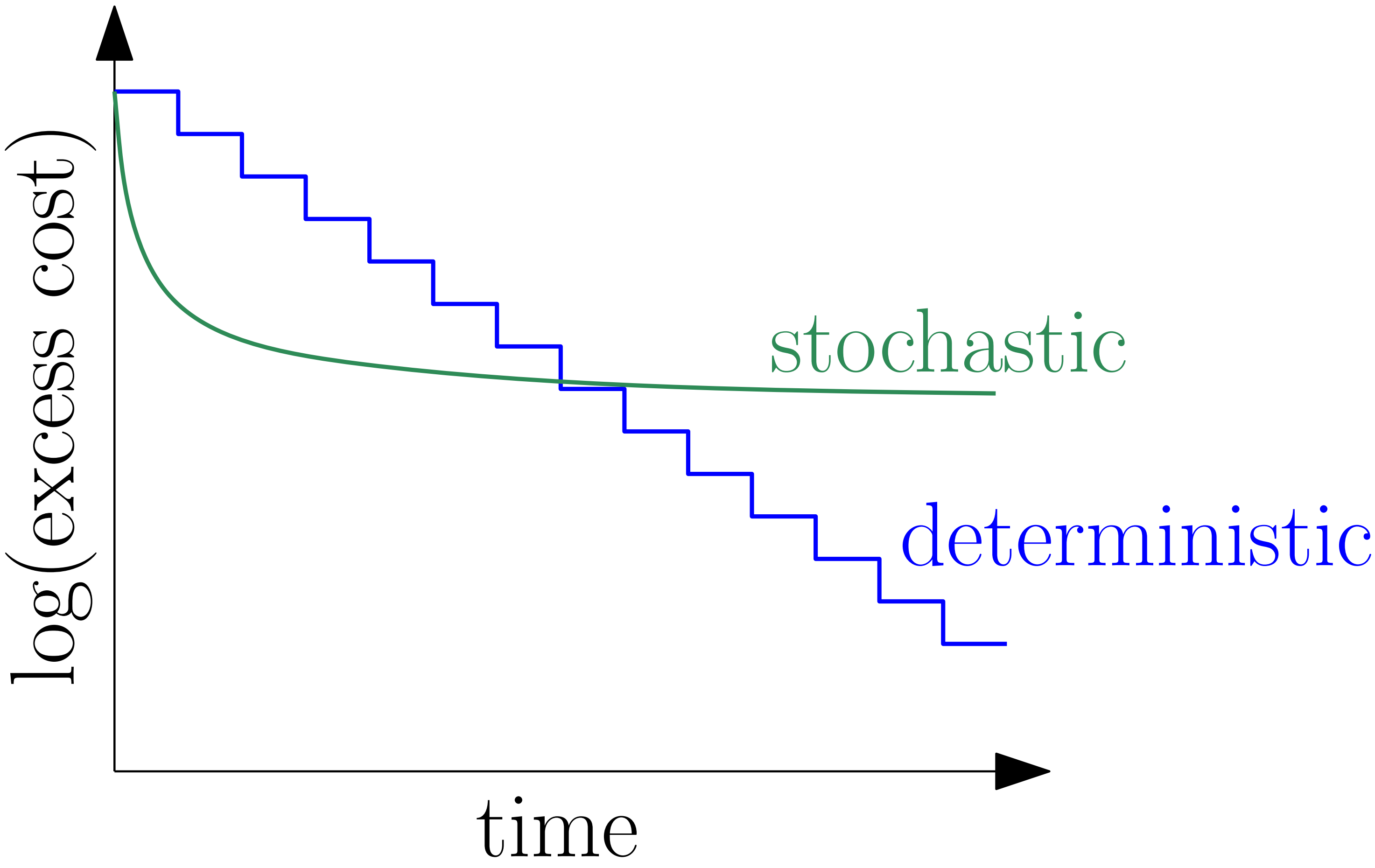


Stochastic vs. deterministic methods

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



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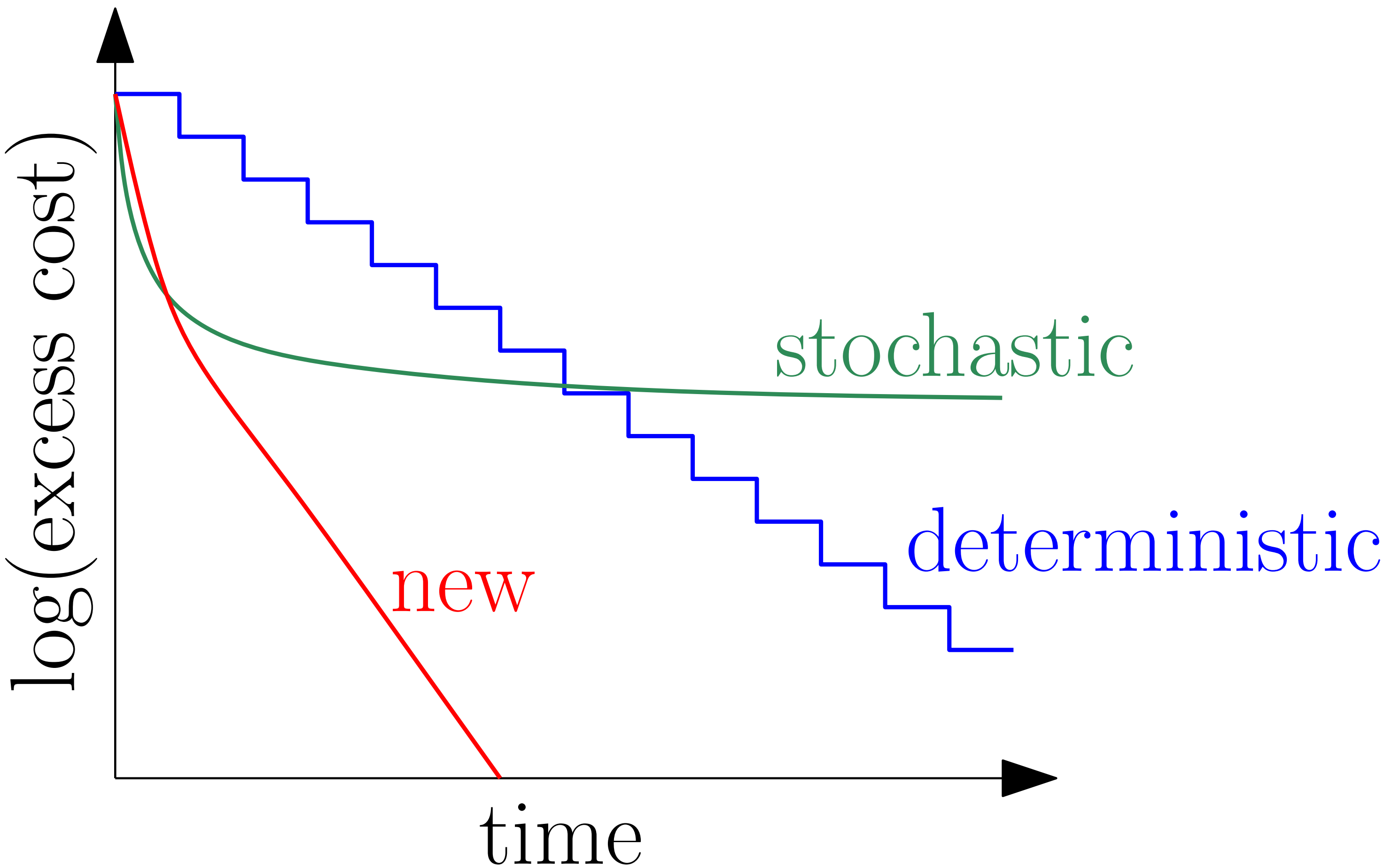

Accelerating gradient methods - Related work

- **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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- **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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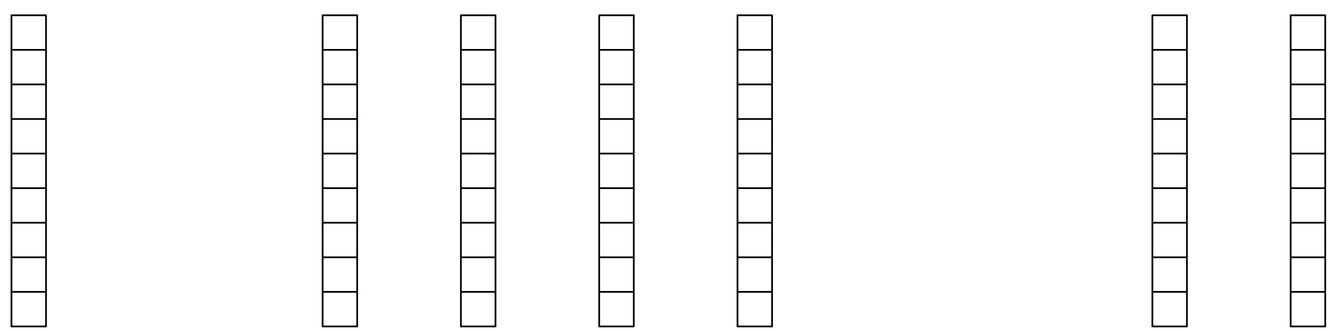
functions	$g = \frac{1}{n}\sum_{i=1}^{n} f_i$	f_1	f_2	f_3	f_4	$\cdots$	f_{n-1}	f_n
gradients $\in \mathbb{R}^d$	$\frac{1}{n}\sum_{i=1}^{n} y_i^t$	y_1^t	y_2^t	y_3^t	y_4^t	$\cdots$	y_{n-1}^t	y_n^t



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  - Keep in memory the gradients of all functions f_i, $i = 1, \dots, n$
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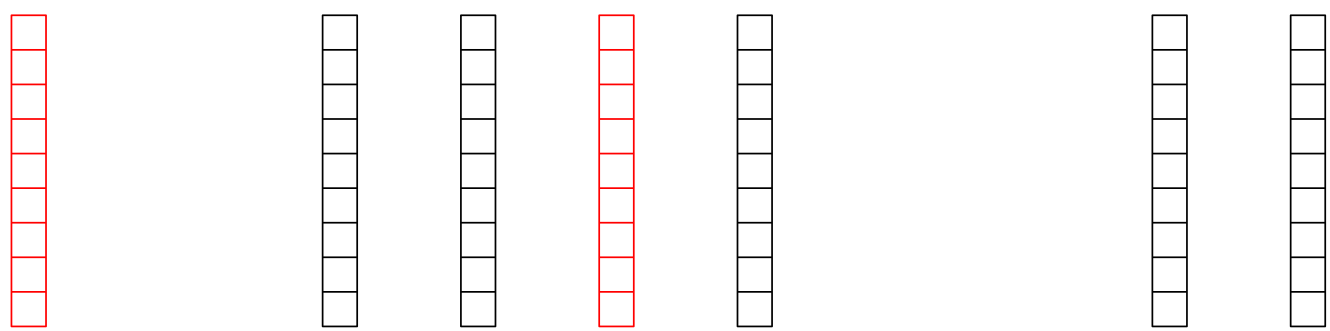
  - Iteration: $\theta_t = \theta_{t-1} - \dfrac{\gamma_t}{n} \displaystyle\sum_{i=1}^{n} y_i^t$ with $y_i^t = \begin{cases} f_i'(\theta_{t-1}) & \text{if } i = i(t) \\ y_i^{t-1} & \text{otherwise} \end{cases}$

functions	$g = \frac{1}{n}\sum_{i=1}^n f_i$	f_1	f_2	f_3	f_4	$\cdots$	f_{n-1}	f_n
gradients $\in \mathbb{R}^d$	$\frac{1}{n}\sum_{i=1}^n y_i^t$	y_1^t	y_2^t	y_3^t	y_4^t	$\cdots$	y_{n-1}^t	y_n^t



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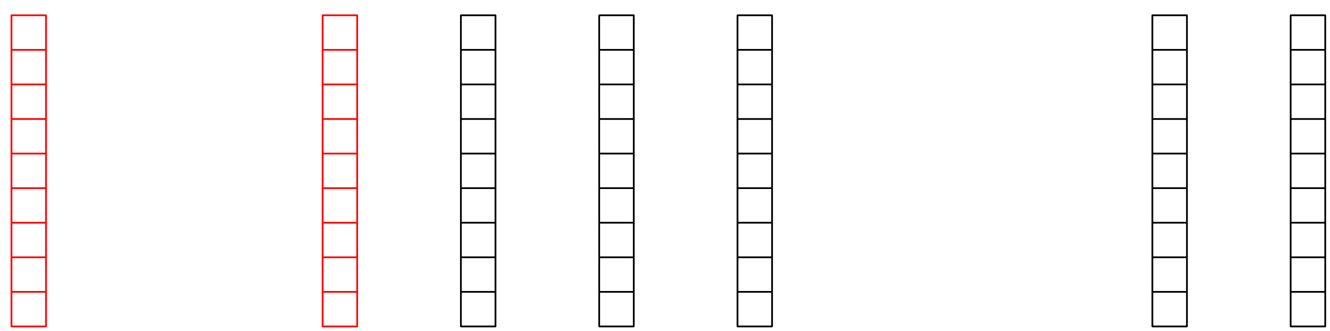

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- Stochastic version of incremental average gradient (Blatt et al., 2008)

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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

Stochastic gradient descent	$d\times$	$\frac{L}{\mu}$	$\times \; \frac{1}{\varepsilon}$
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	$d\times$	$(n + \frac{L}{\mu})$	$\times \log \frac{1}{\varepsilon}$

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

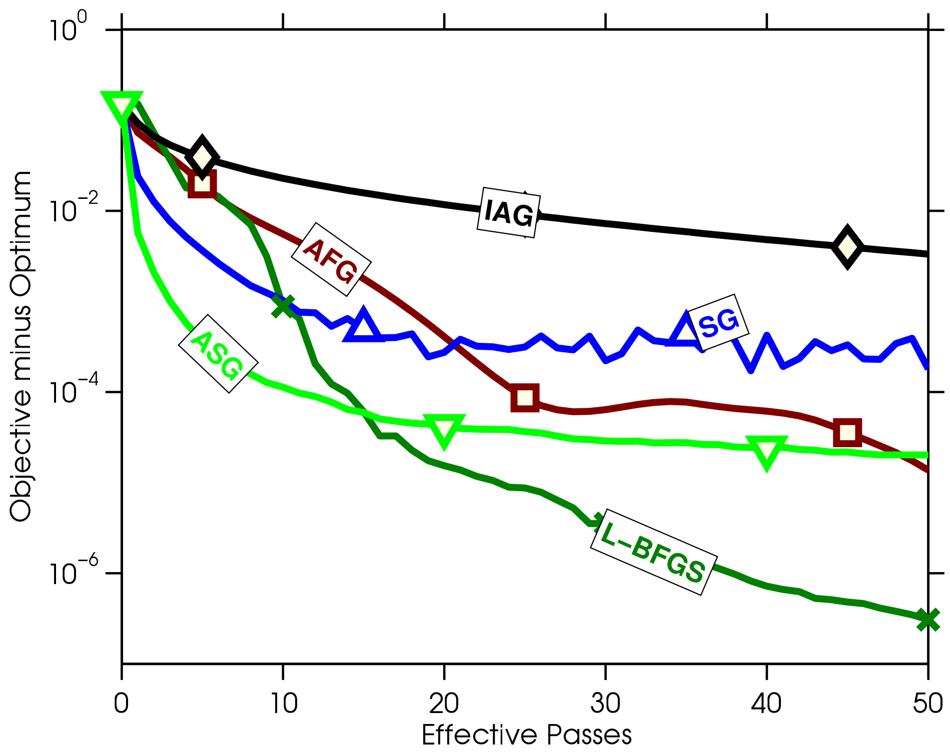
Stochastic average gradient
Implementation details and extensions

- **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)

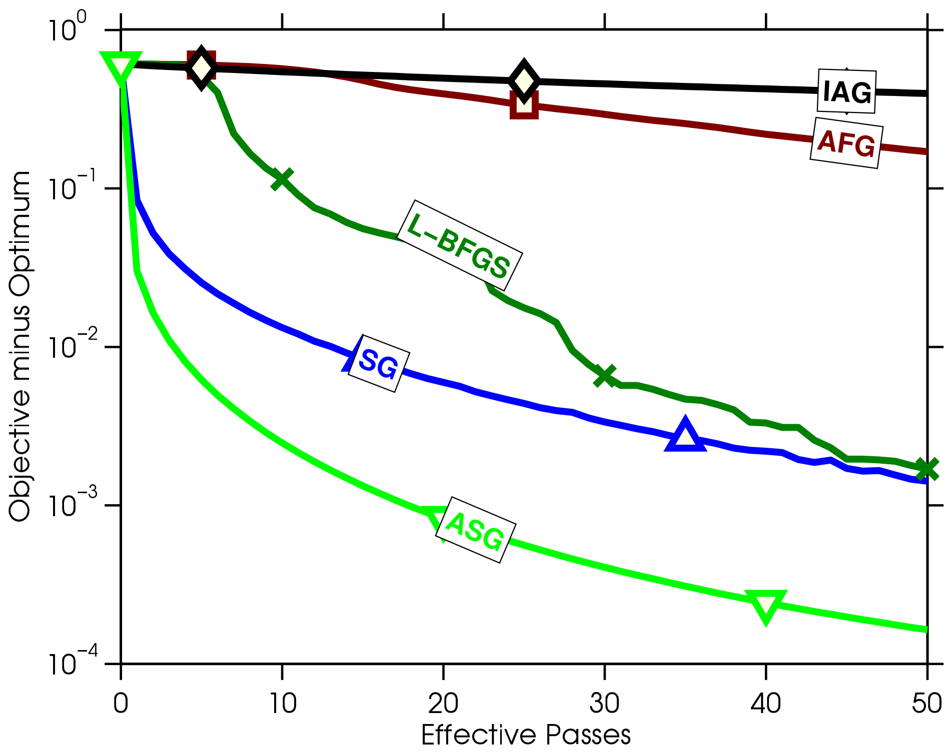
`quantum` dataset

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



`rcv1` dataset

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



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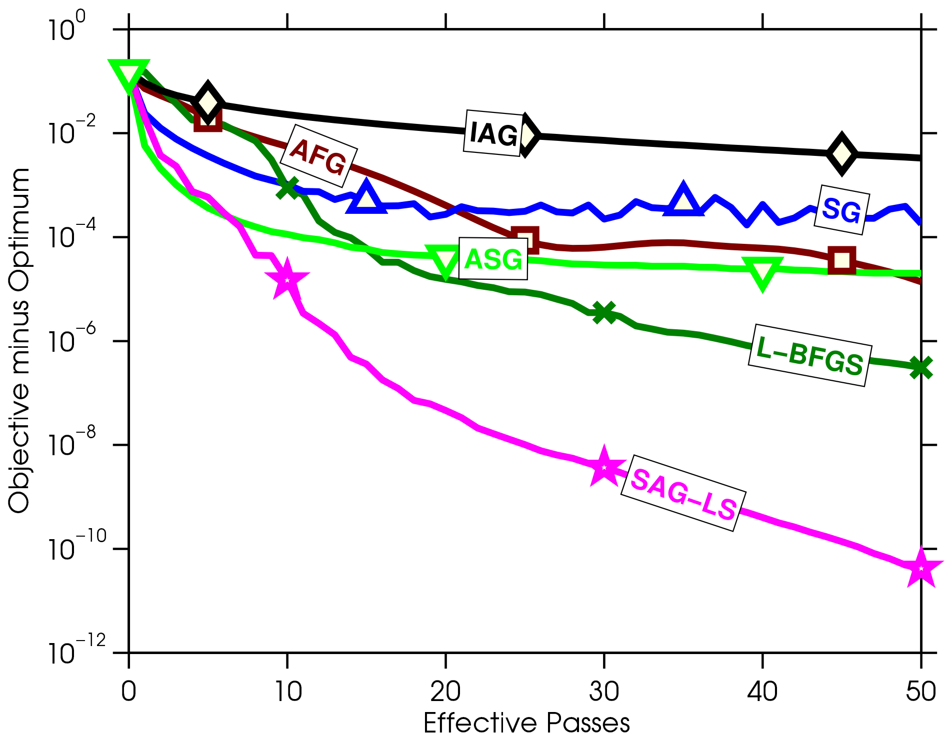
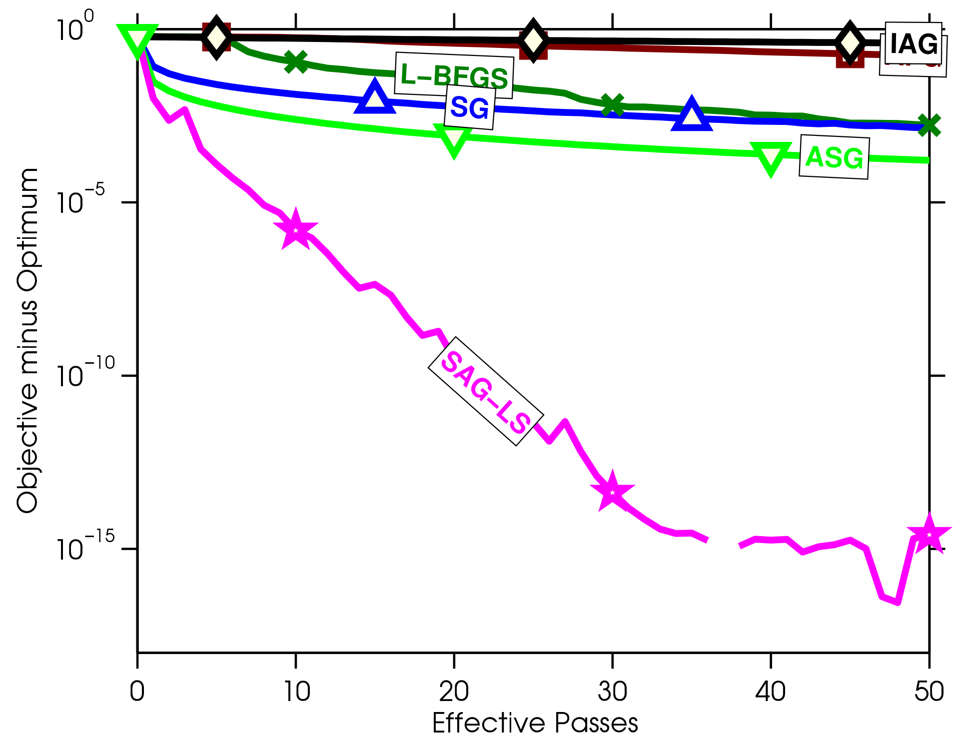
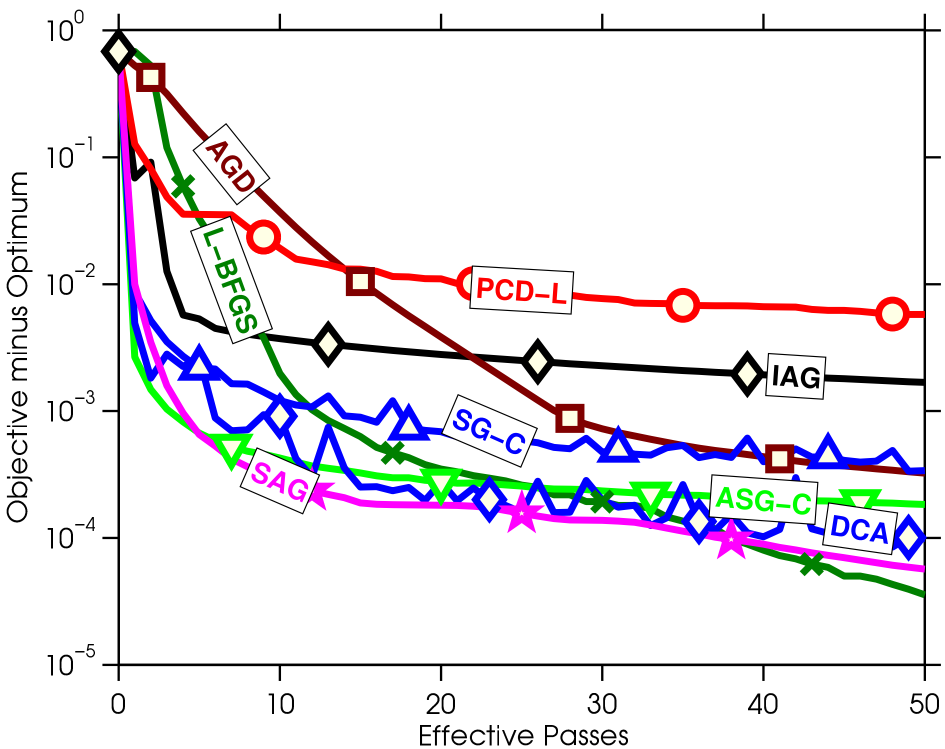


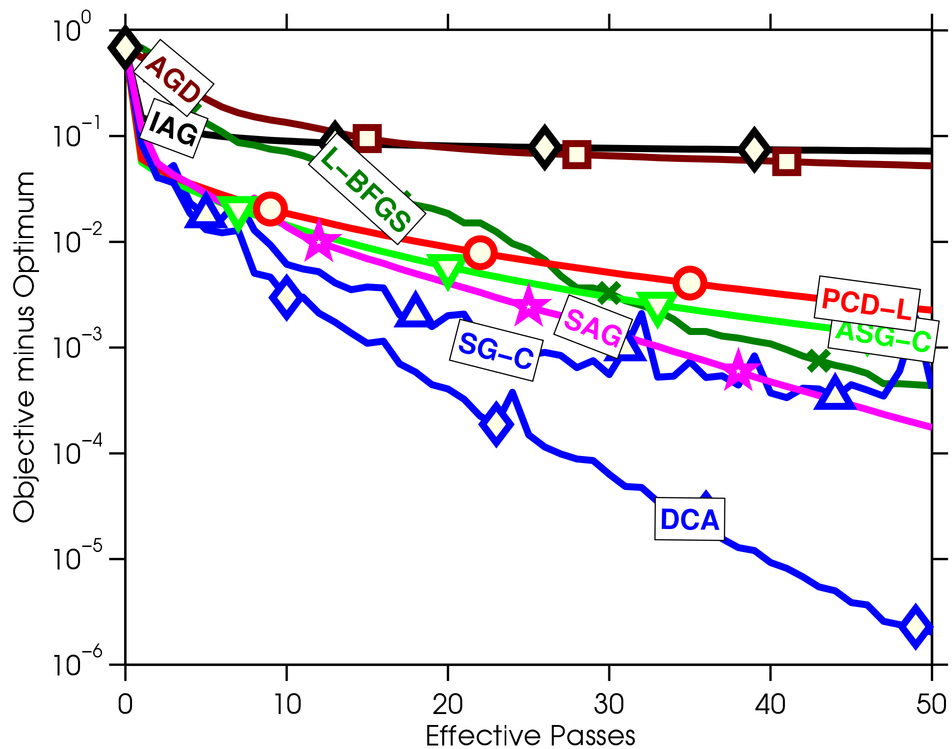


Before non-uniform sampling

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



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



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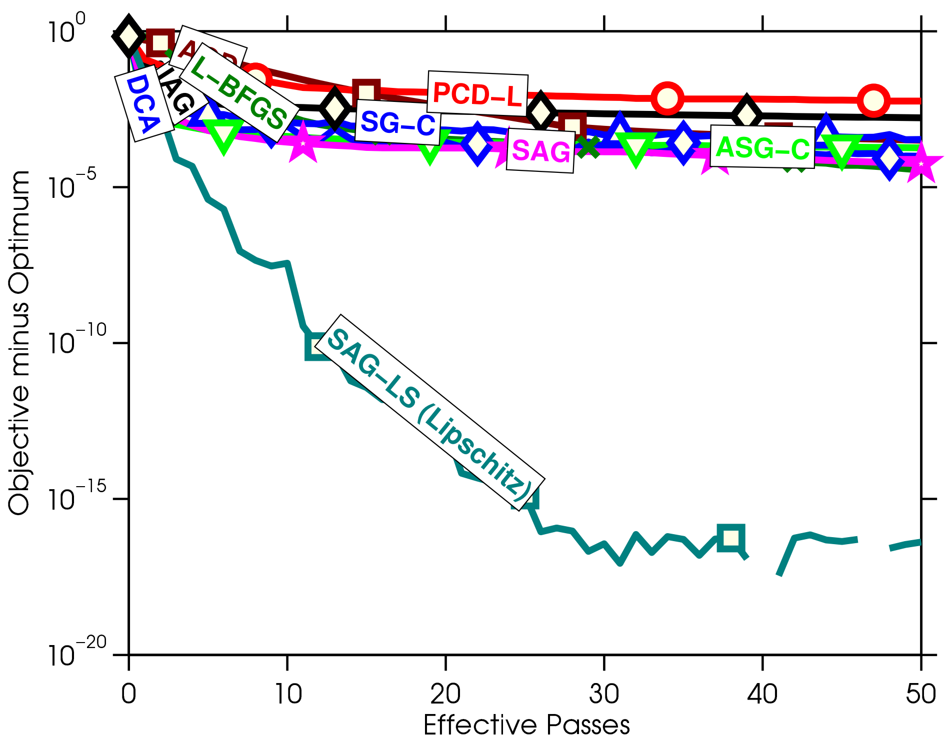

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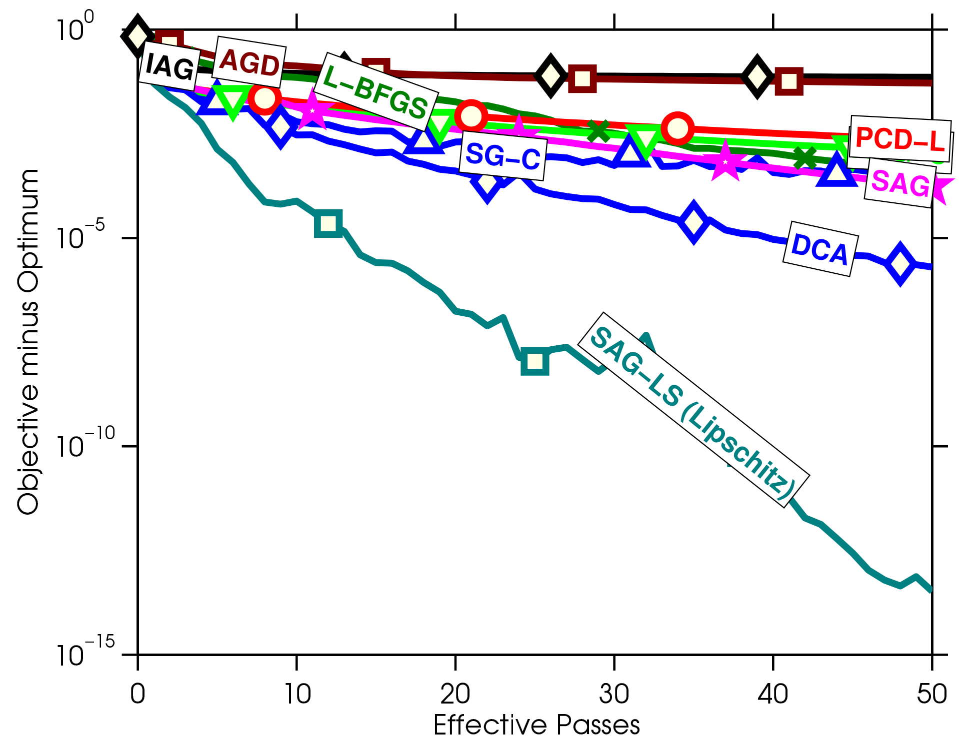
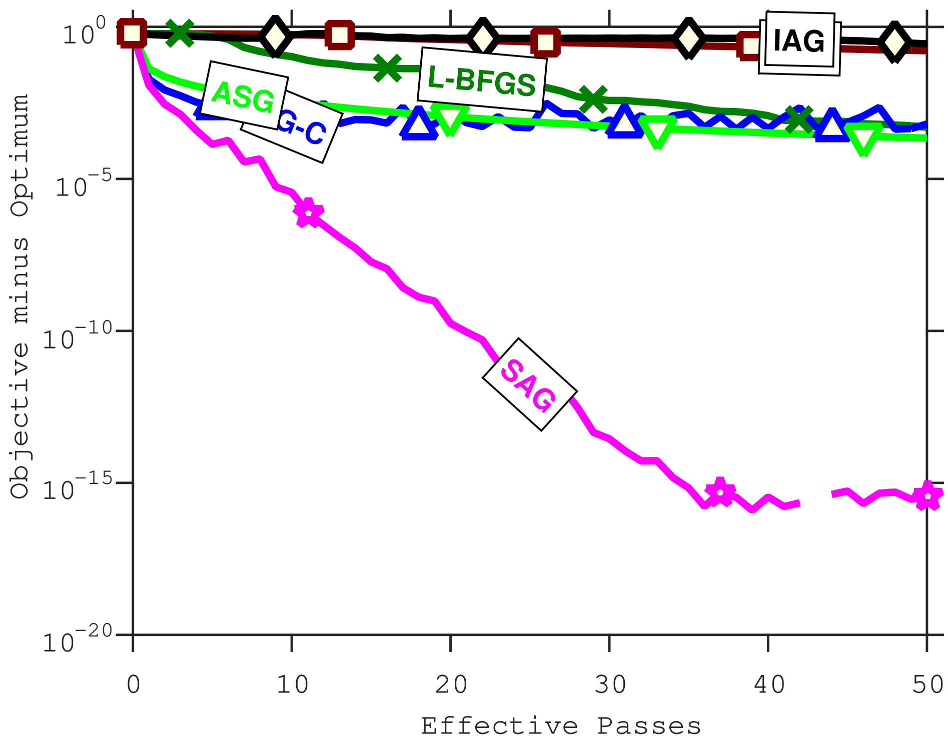


From training to testing errors

- 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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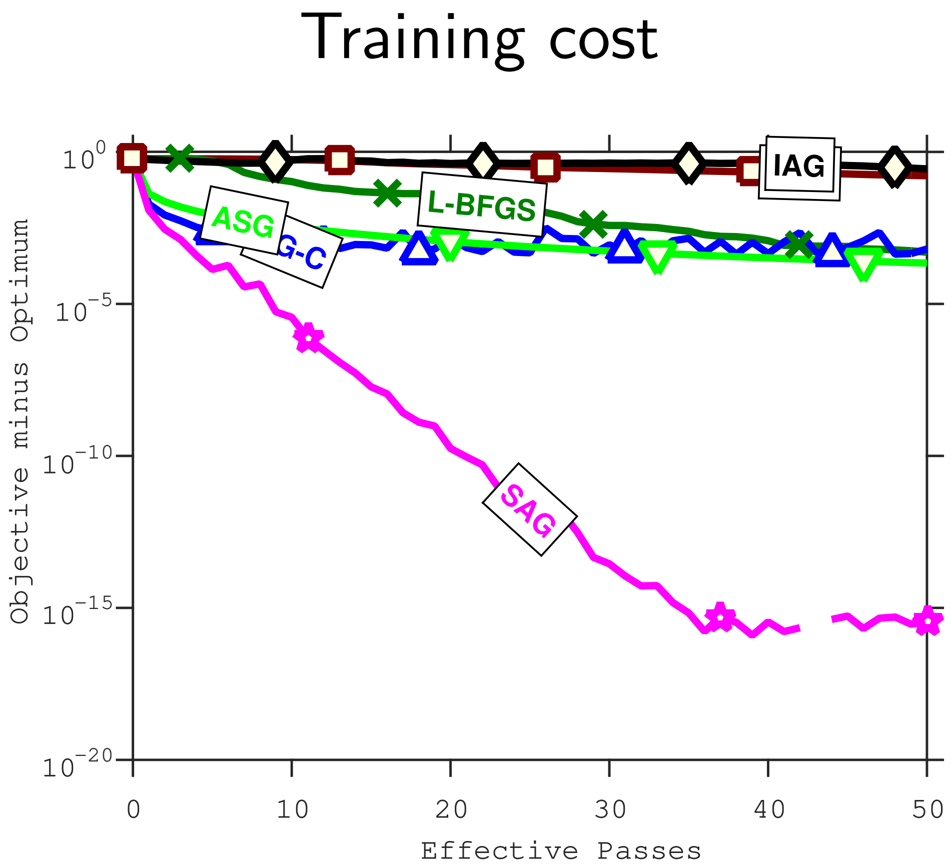

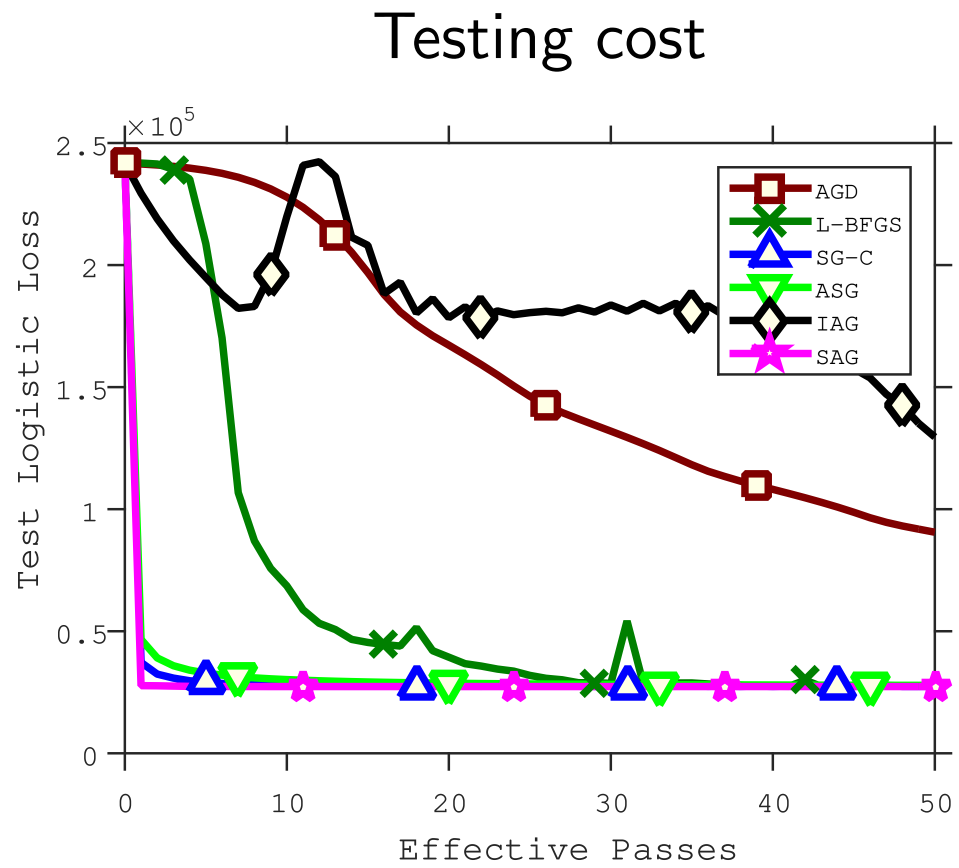

Linearly convergent stochastic gradient algorithms

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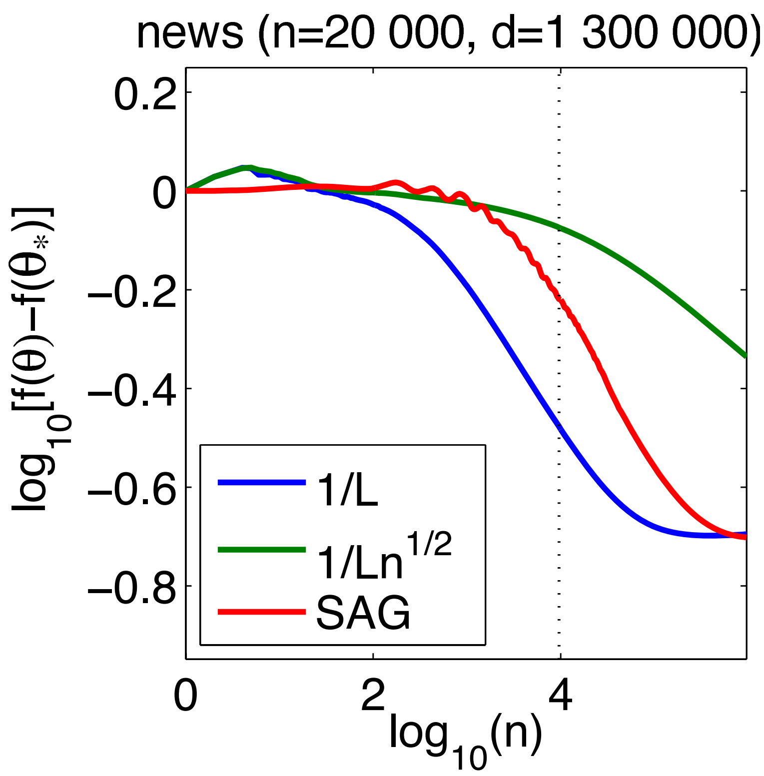
- **Constant-step-size SGD**
  - Linear convergence up to the noise level for strongly-convex problems (Solodov, 1998; Nedic and Bertsekas, 2000)
  - Full convergence and robustness to ill-conditioning?

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)*

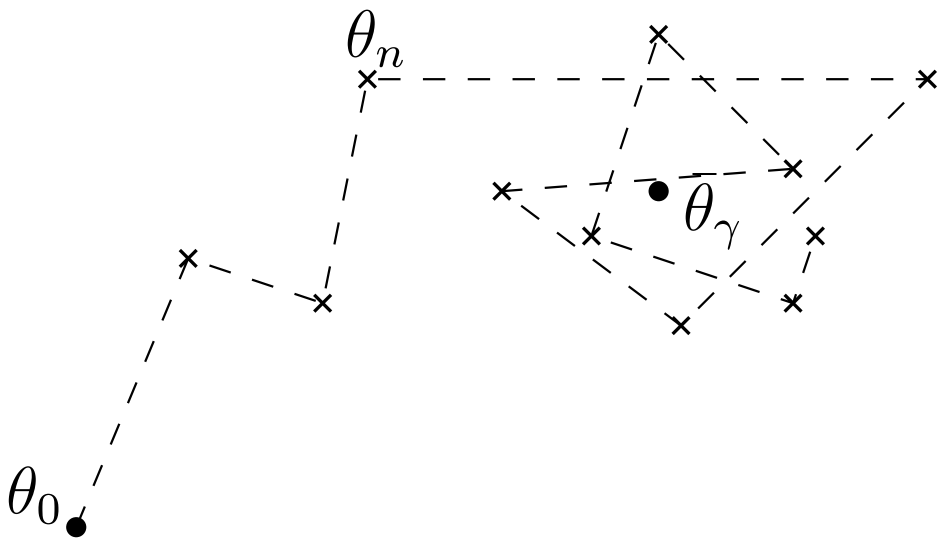


Markov chain interpretation of constant step sizes

- 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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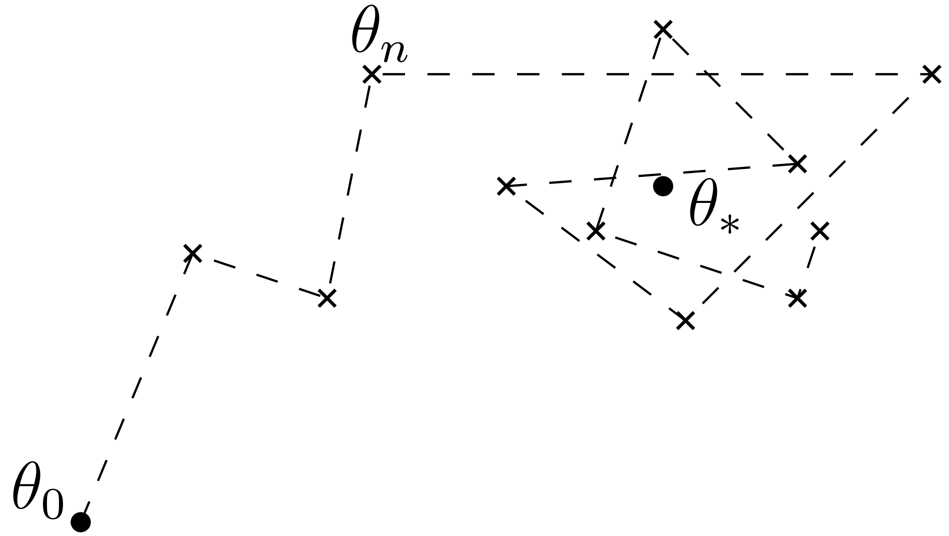

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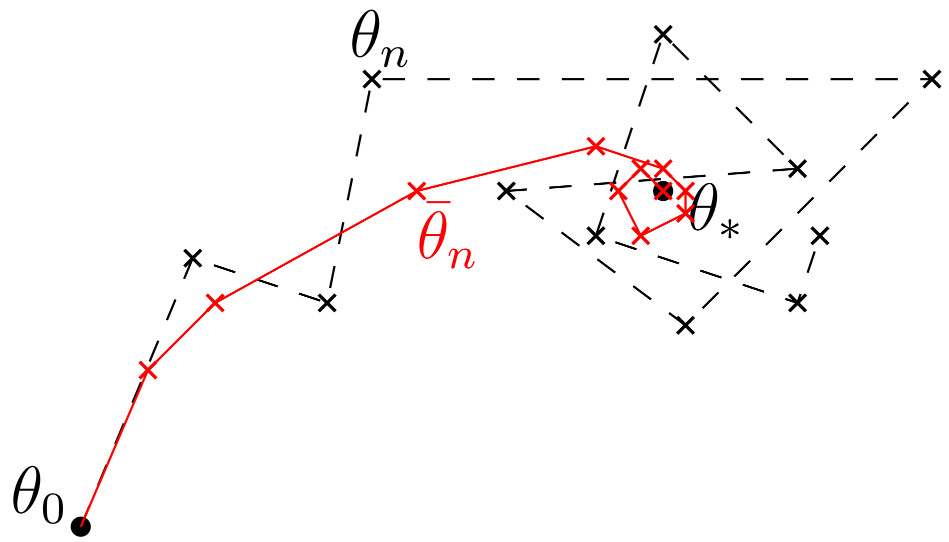

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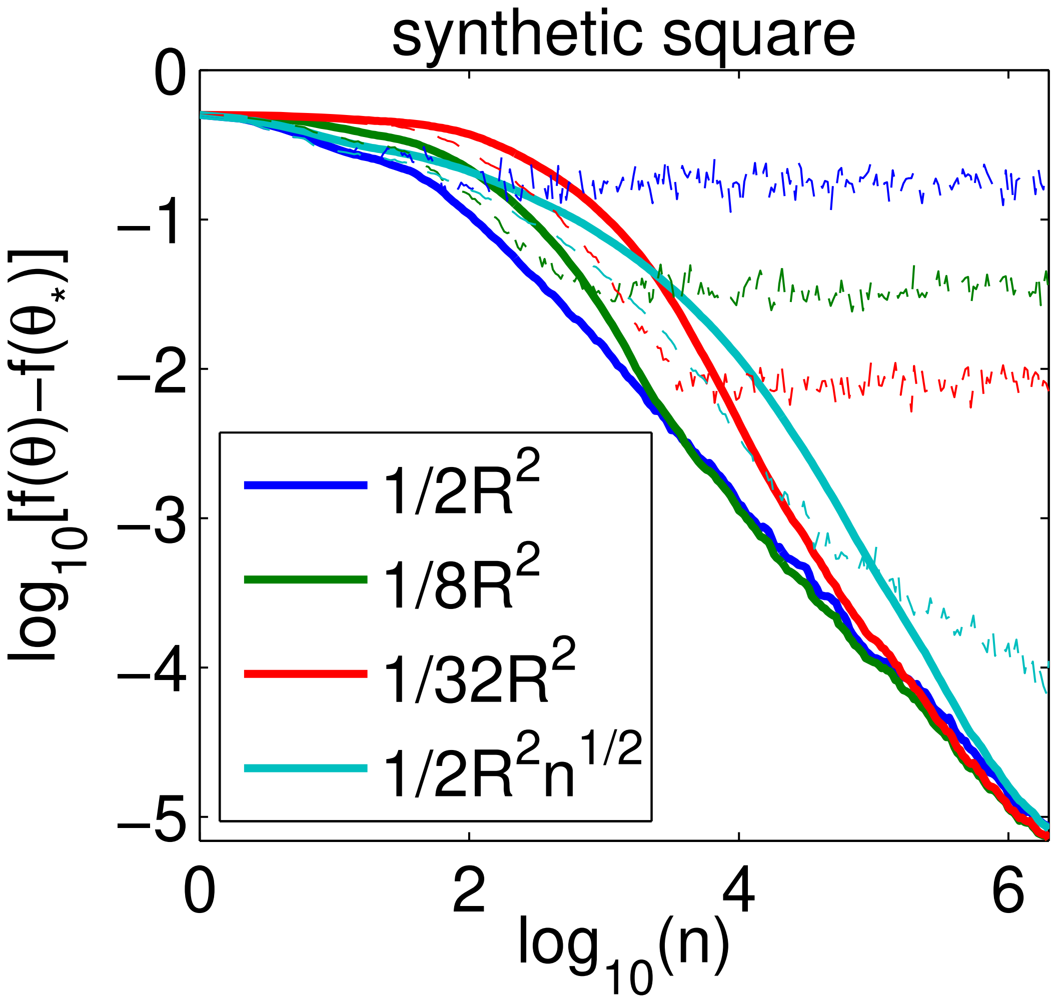
  - θ_n does not converge to θ_* but oscillates around it
  - oscillations of order $\sqrt{\gamma}$

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

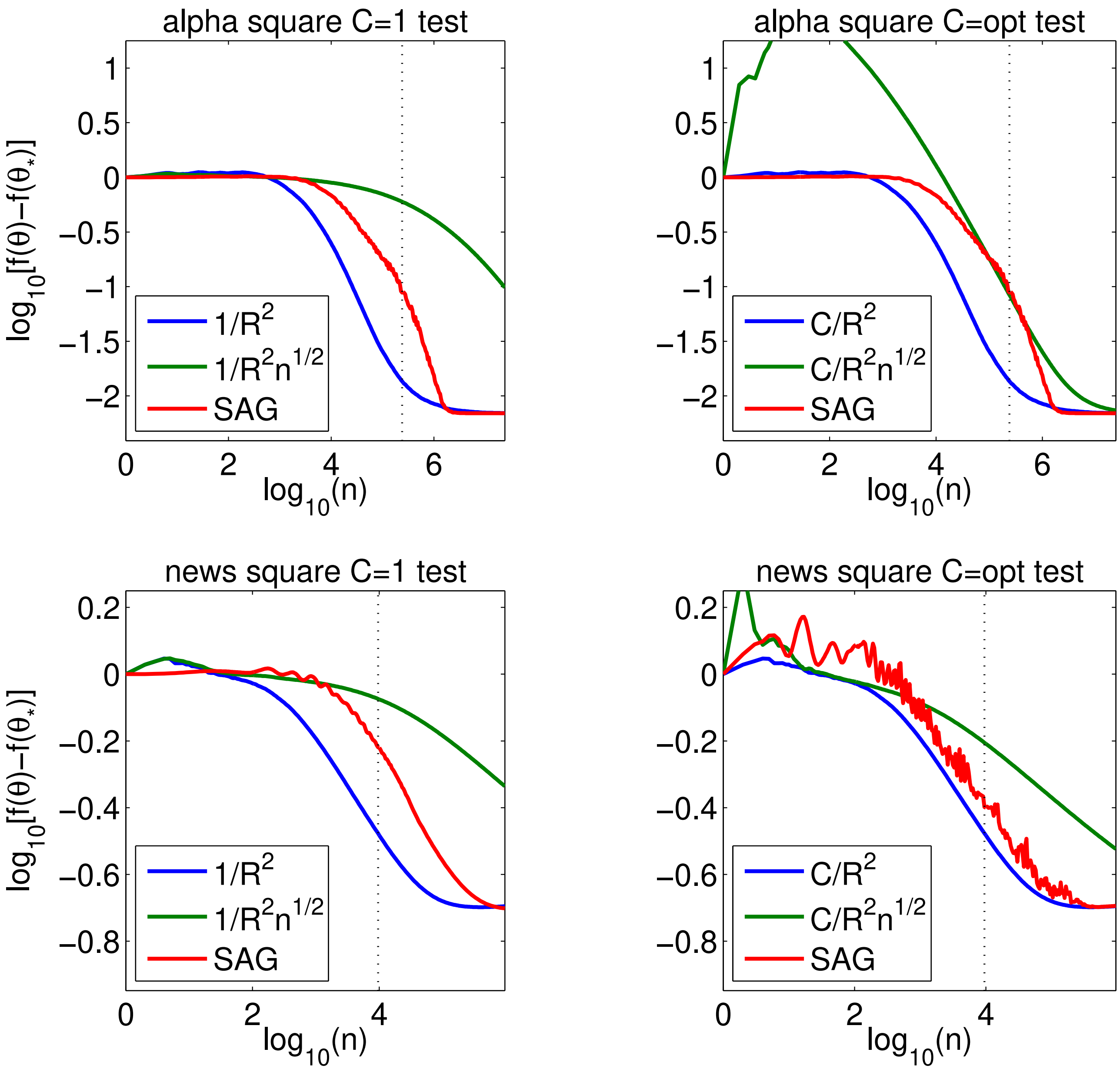
Simulations - synthetic examples

- Gaussian distributions - $p = 20$



Simulations - benchmarks

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



Robust averaged stochastic gradient (Bach and Moulines, 2013)

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  - Online Newton correction with same complexity as SGD
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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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  - Parallelization (Leblond, Pedregosa, and Lacoste-Julien, 2016; Hendrikx, Bach, and Massoulié, 2019)
  - Non-convex problems (Reddi et al., 2016)
  - Other forms of acceleration (Scieur, d'Aspremont, and Bach, 2016)

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**:

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

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)
  - 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), etc...

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

Exponentially convergent SGD for finite sums

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

Stochastic gradient descent	$d\times$	κ	$\times$	$\frac{1}{\varepsilon}$
Gradient descent	$d\times$	$n\kappa$	$\times$	$\log \frac{1}{\varepsilon}$
Accelerated gradient descent	$d\times$	$n\sqrt{\kappa}$	$\times$	$\log \frac{1}{\varepsilon}$

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NB: slightly different (smaller) notion of condition number for batch methods

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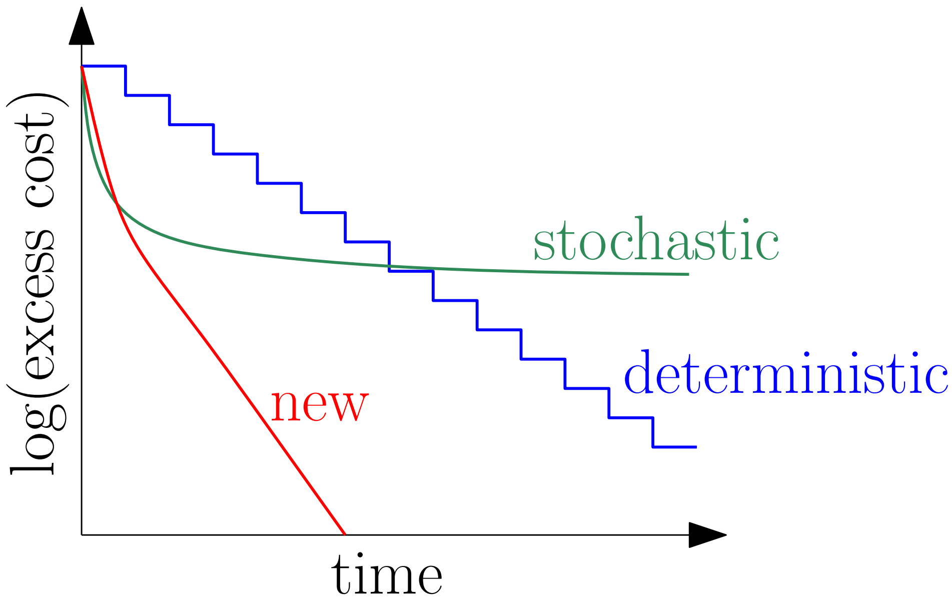
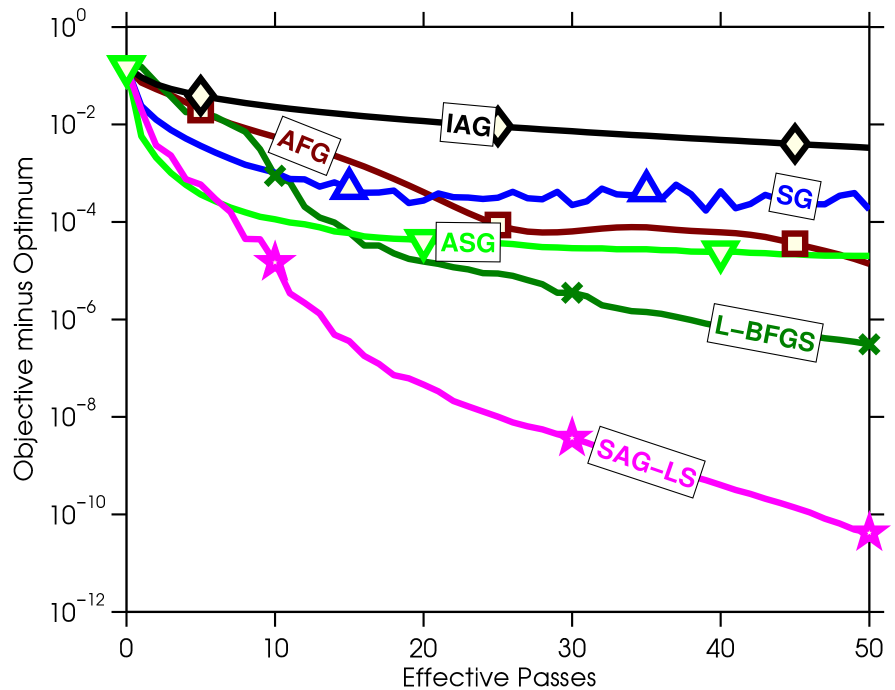
- **Matching lower bounds** (Woodworth and Srebro, 2016; Lan, 2015)

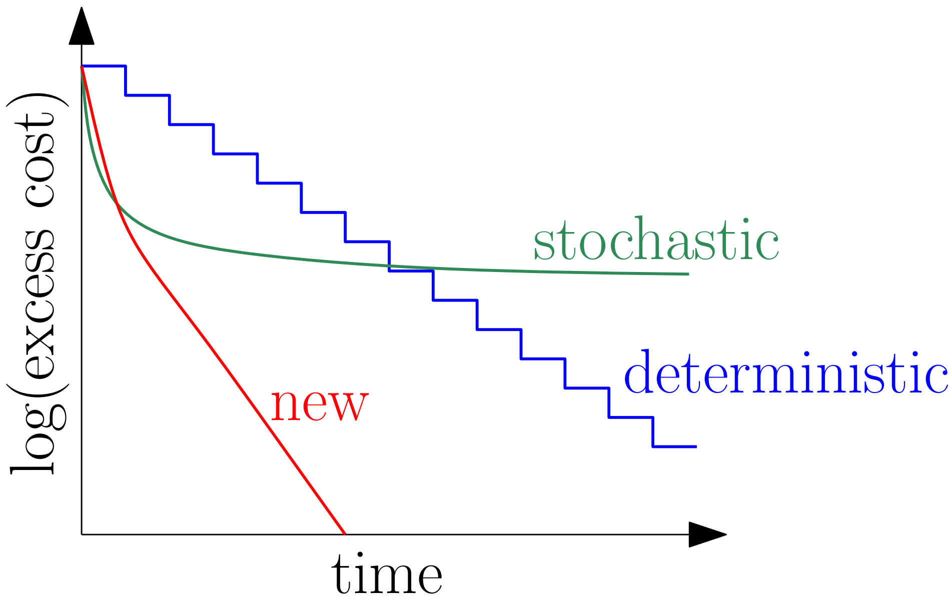
Exponentially convergent SGD for finite sums
From theory to practice and vice-versa

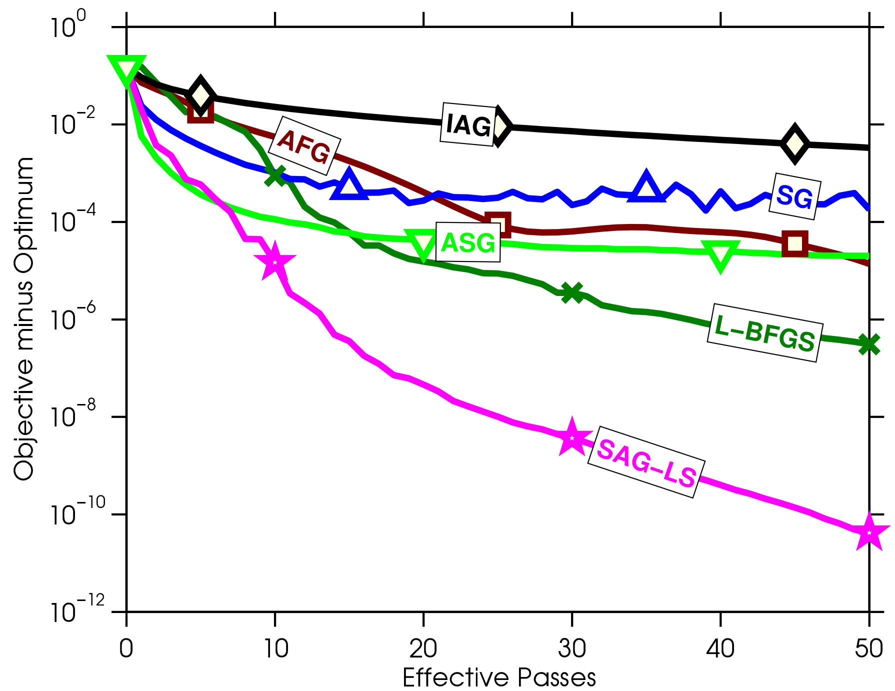




- **Empirical performance "matches" theoretical guarantees**

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

- **Empirical performance "matches" theoretical guarantees**
- **Theoretical analysis suggests practical improvements**
- **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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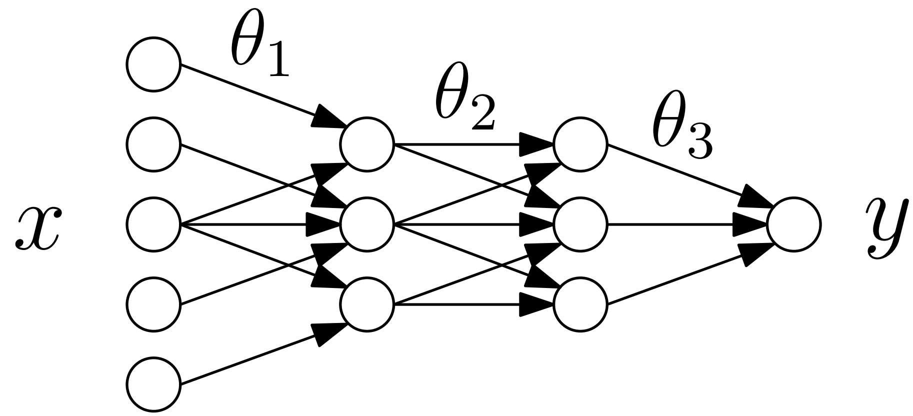
- **What about deep learning?**

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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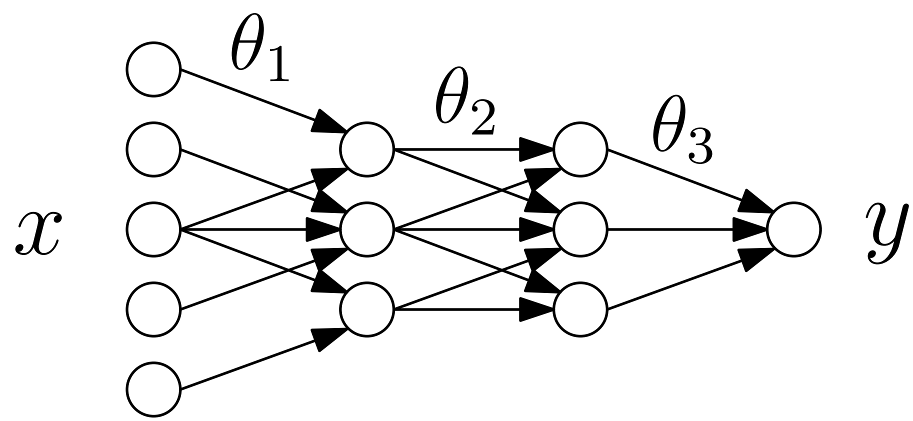

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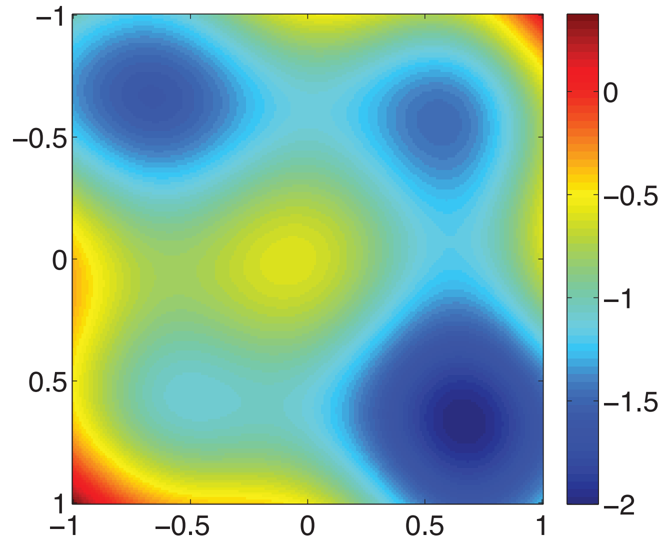
- **Main difficulties**

  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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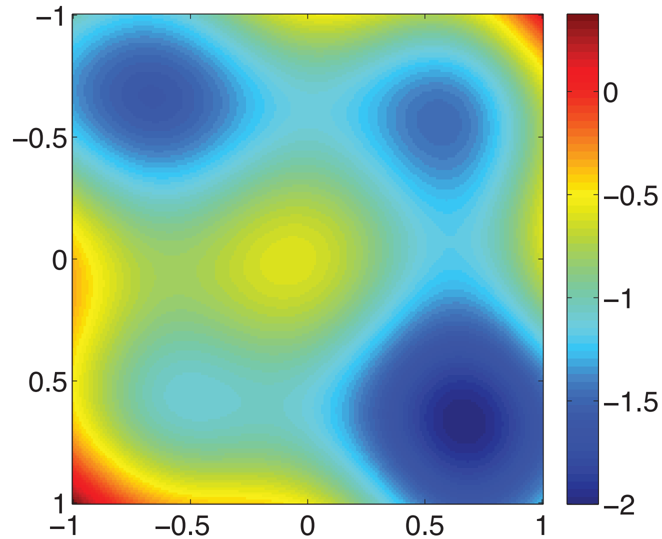

- **Generic local theoretical guarantees**

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

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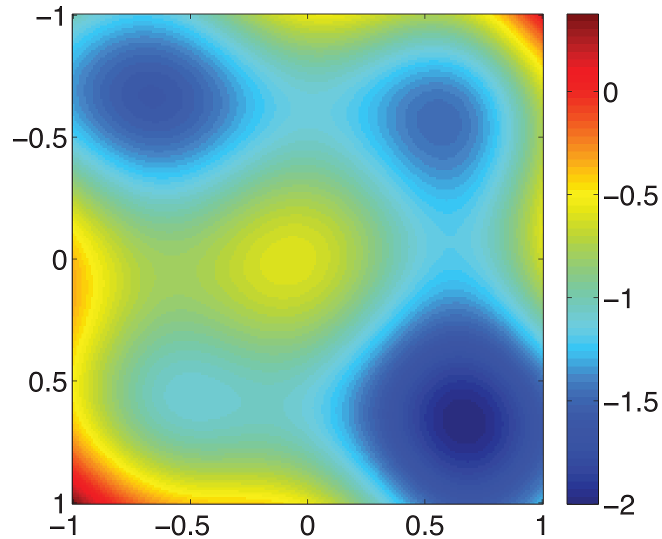

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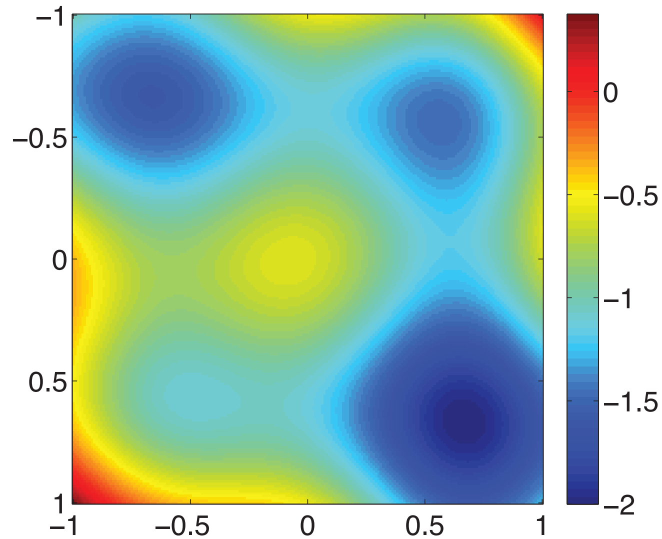

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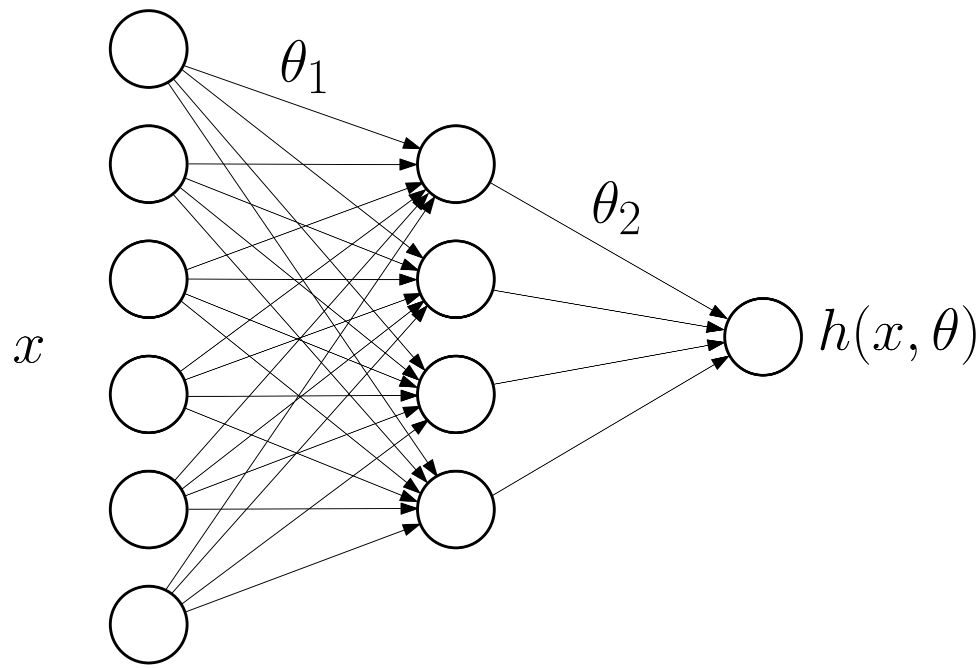
- **Special case of (deep) neural networks**
  - Most local minima are equivalent (Choromanska et al., 2015)
  - No spurrious local minima (Soltanolkotabi et al., 2018)

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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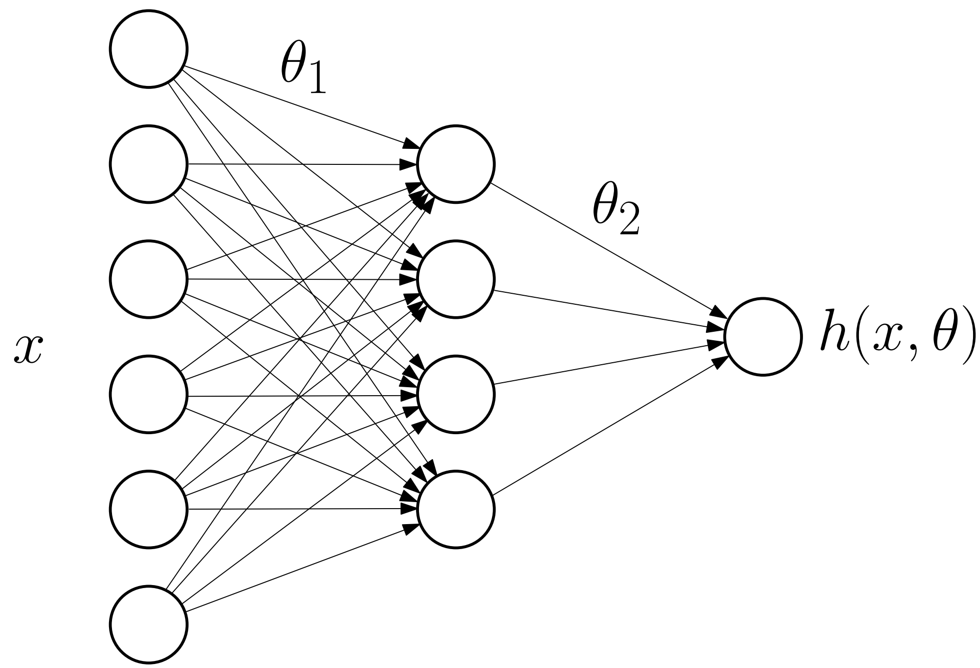

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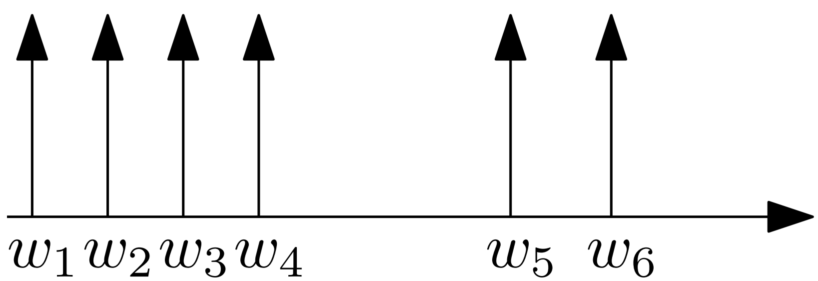
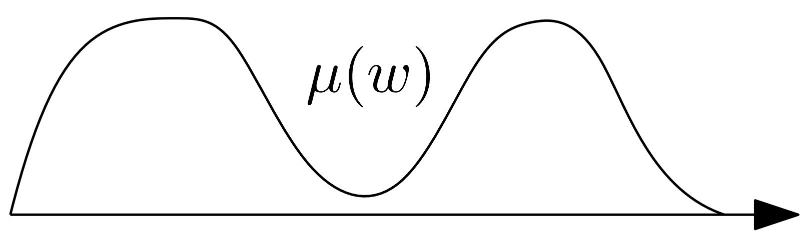
- **Main insight**
  - $h = \dfrac{1}{m}\displaystyle\sum_{j=1}^m \Psi(w_j) = \int_{\mathcal{W}} \Psi(w) d\mu(w)$ with $d\mu(w) = \dfrac{1}{m}\displaystyle\sum_{j=1}^m \delta_{w_j}$





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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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    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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  - 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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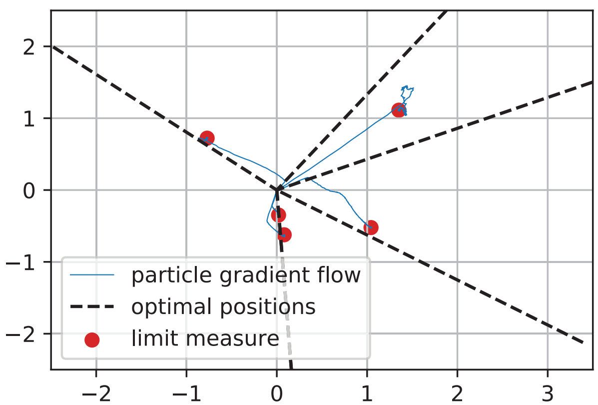
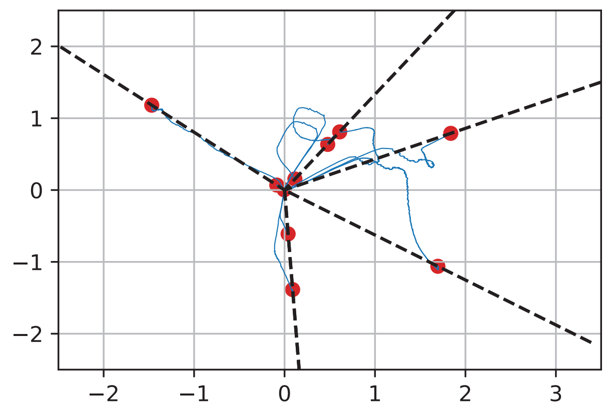
- **Only qualititative!**

Simple simulations with neural networks

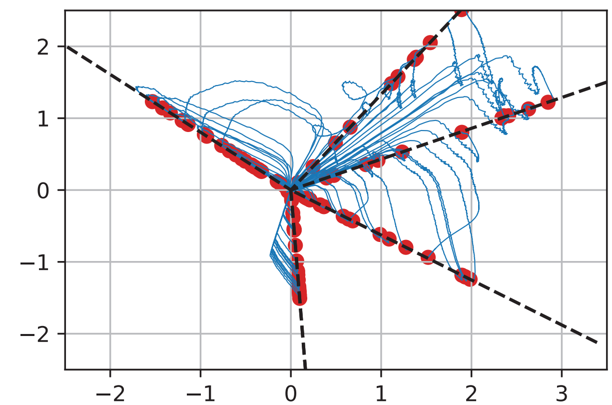
- ReLU units with $d = 2$ (optimal predictor has 5 neurons)



5 neurons



10 neurons



100 neurons

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

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

NB : also applies to spike deconvolution

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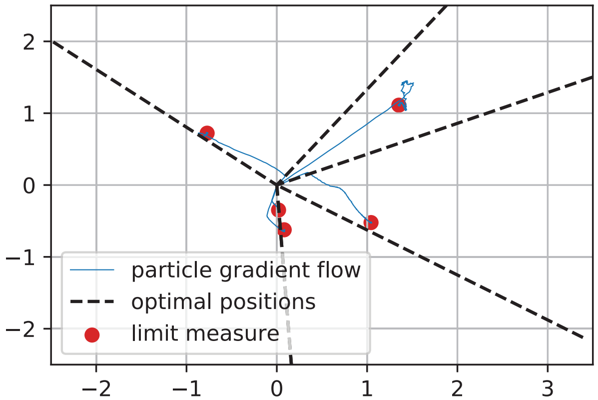

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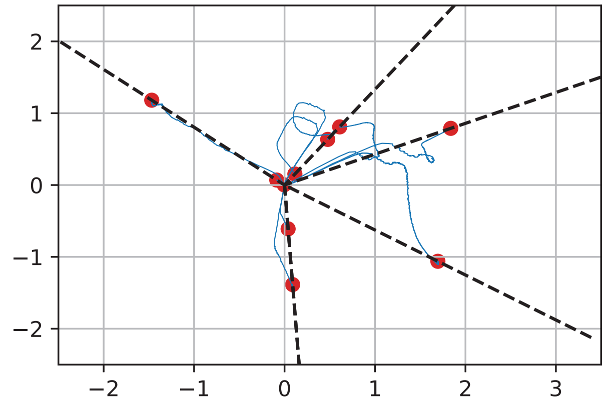

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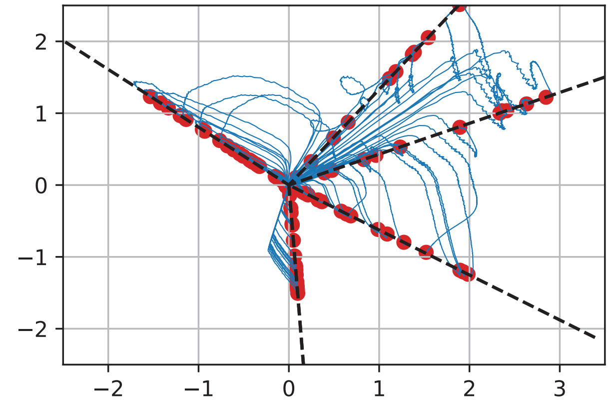

100 neurons

video!

NB : also applies to spike deconvolution

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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  - `https://arxiv.org/abs/1811.03804`
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- **Any link?**

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- **Recent bursty activity on ArXiv**
  - Corresponds to initializing with weights which are $\sqrt{m}$ times larger
  - Where does it converge to?

From qualitative to quantitative results ?

- **Mean-field limit**: $h(W) = \frac{1}{m}\sum_{i=1}^{m} \Psi(w_i)$
  - With w_i initialized randomly (with variance independent of m)
  - Dynamics equivalent to Wasserstein gradient flow
  - Convergence to global minimum of $R(\int \Psi d\mu)$
- **Recent bursty activity on ArXiv**
  - Corresponds to initializing with weights which are $\sqrt{m}$ times larger
  - Where does it converge to?
- **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
    (using, e.g., $\mathbb{E}\Psi(w_i) = 0$)

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

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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

$$\|W(t) - W(0)\| = O(1/\alpha) \text{ and } \alpha h(W(t)) \to \arg\min_h R(h) \text{ “linearly”}$$

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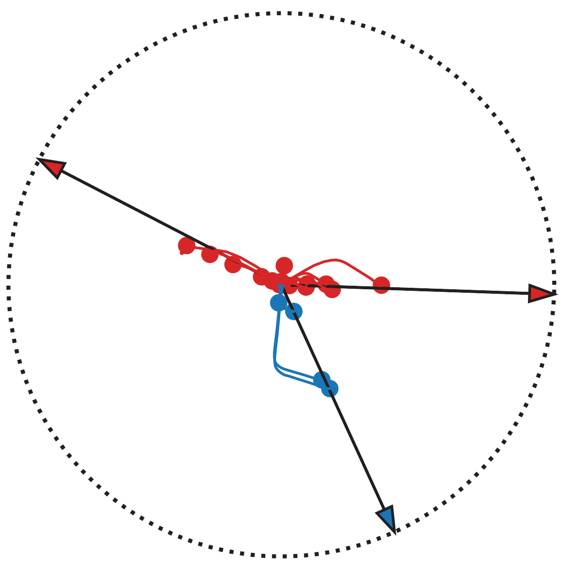

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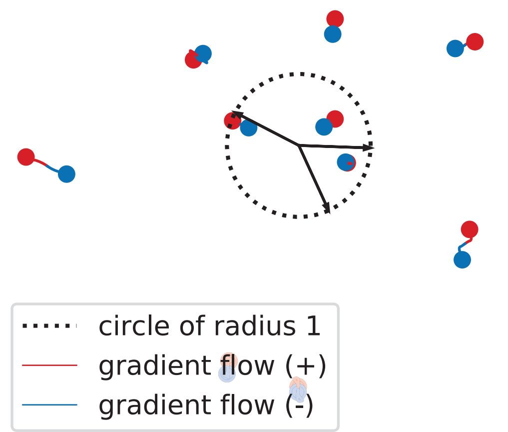

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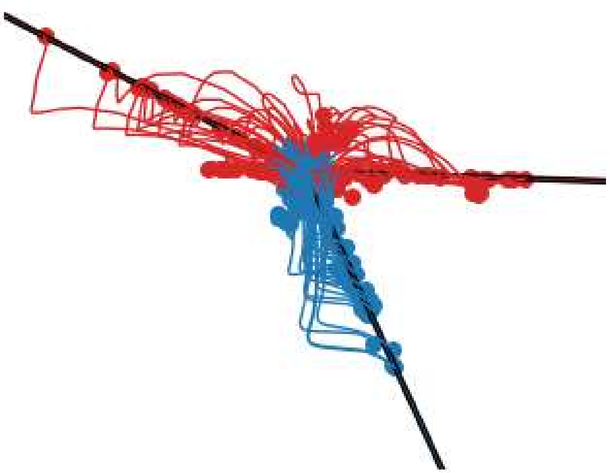

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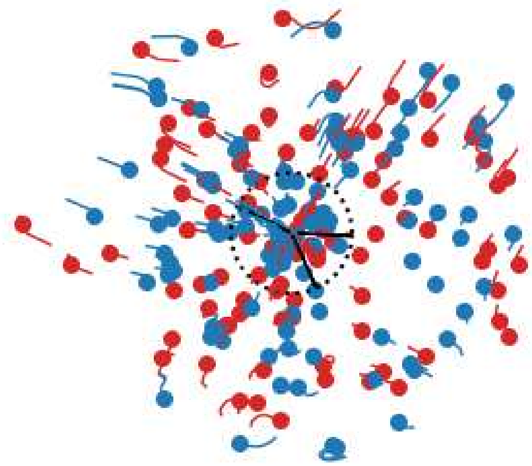

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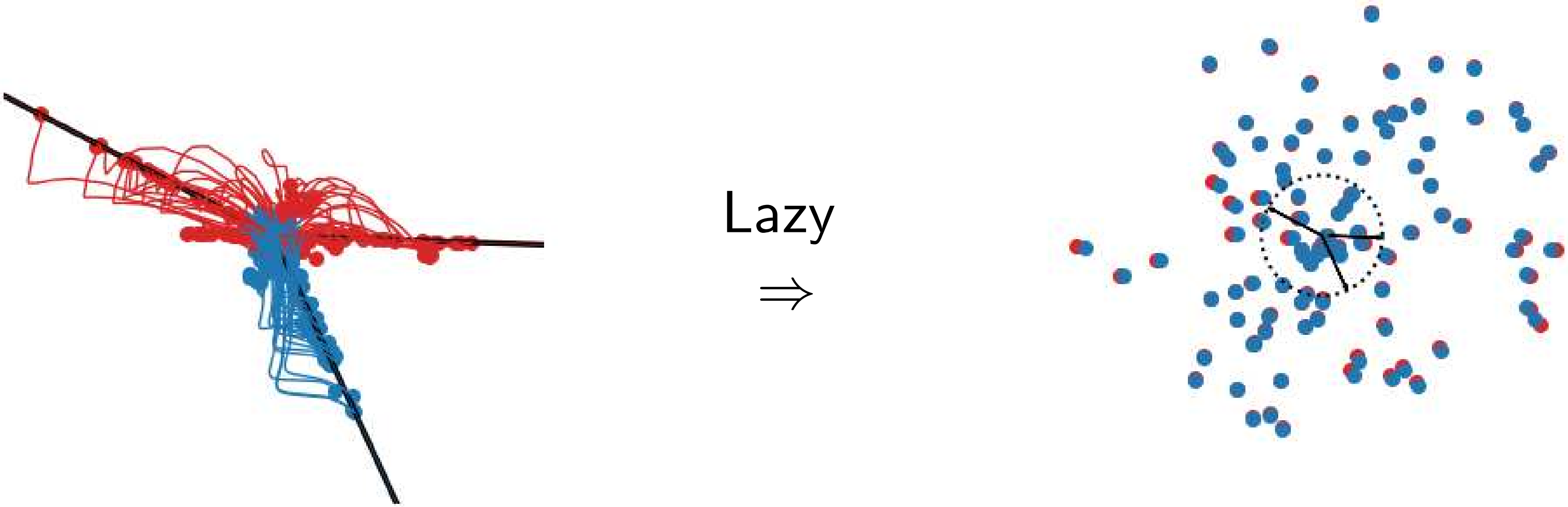

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$\Rightarrow$ Equivalent to a linear model
$h(W) \approx h(W(0)) + (W - W(0))^\top \nabla h(W(0))$

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?

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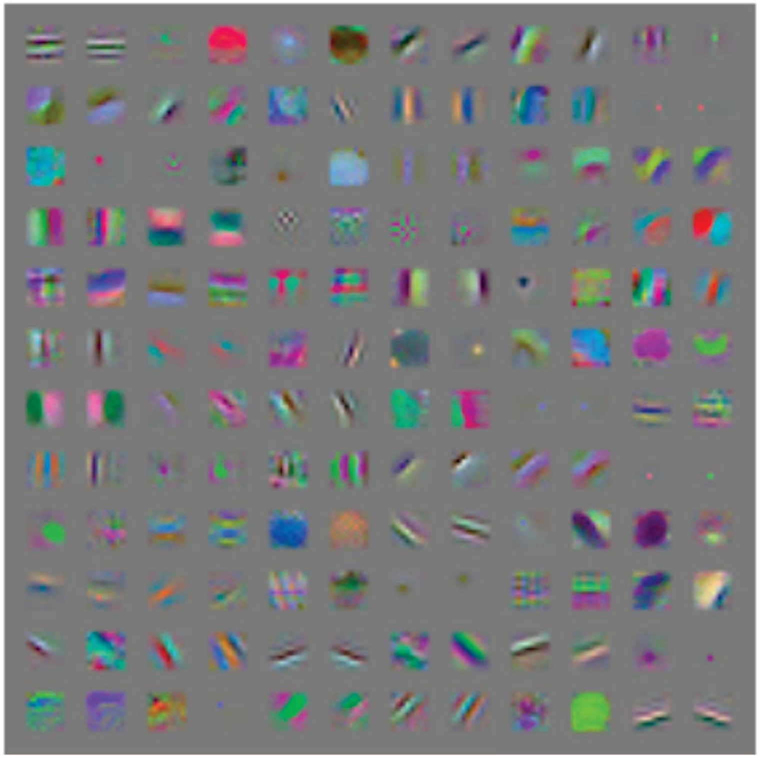

From Goodfellow, Bengio, and Courville (2016)

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

- **Lazy regime**: Neurons move infinitesimally
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- **Evidence 2**, by Zhang et al. (2019)
  - Neurons from first layers do move
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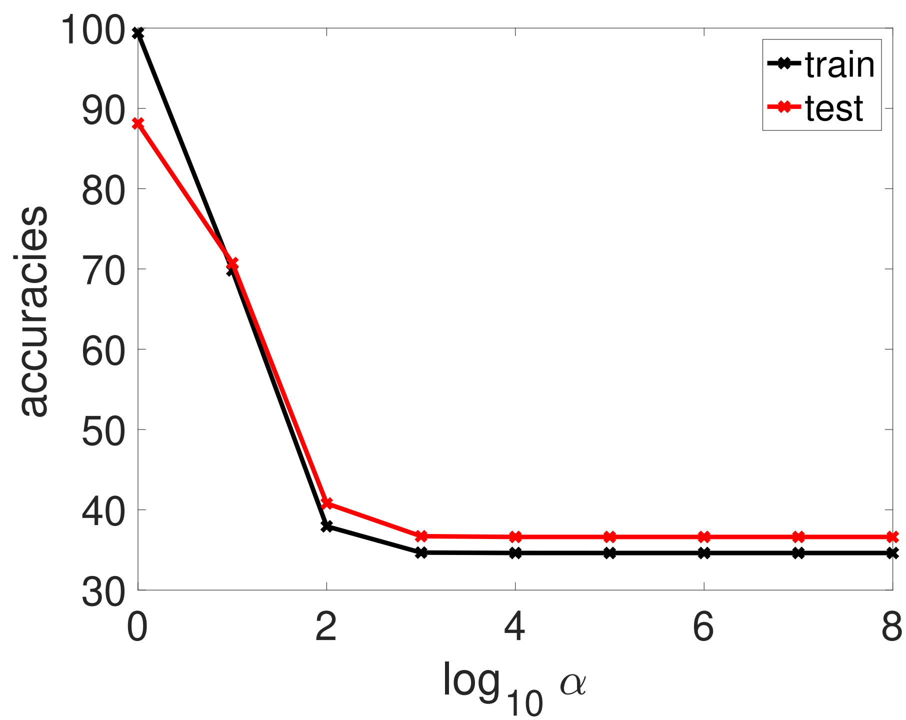
- **Evidence 3**: Take a state-of-the-art CNN and make it lazier
  - Chizat, Oyallon, and Bach (2019)

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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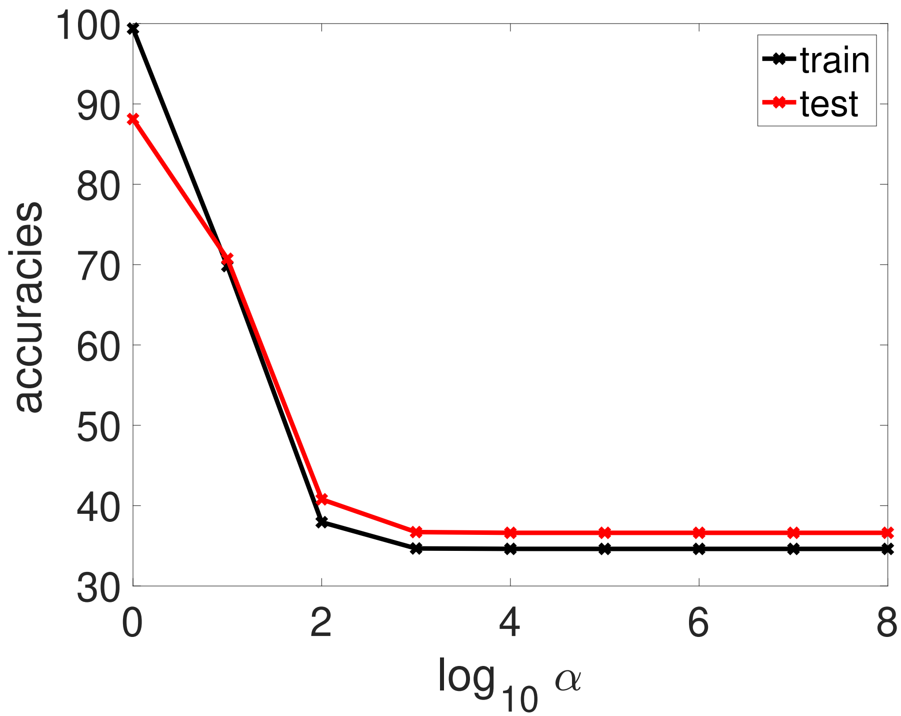

- **Understanding the mix of lazy and non-lazy regimes?**

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
  - Non-parametric estimation but no better than usual kernels (Ghorbani et al., 2019; Bietti and Mairal, 2019)

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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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- **Empirical successes of deep learning cannot be ignored**

Healthy interactions between theory, applications, and hype?

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

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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  - 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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