

# Stochastic Algorithms in Machine Learning

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ÉCOLE POLYTECHNIQUE  
FÉDÉRALE DE LAUSANNE

# Outline

1. Machine learning context.
2. Stochastic algorithms to minimize **Empirical Risk** .
3. Stochastic Approximation: using stochastic gradient descent (SGD) to minimize **Generalization Risk**.
4. **Markov chain**: insightful point of view on constant step size Stochastic Approximation.

# Supervised Machine Learning

Goal: predict a phenomenon from “explanatory variables”, given a set of observations.



Bio-informatics

Input: DNA/RNA sequence,  
Output: Disease predisposition  
/ Drug responsiveness  
 $n \rightarrow 10$  to  $10^4$   
 $d$  (e.g., number of basis)  
 $\rightarrow 10^6$

```
0 1 2 3 4 5 6 7 8 9
0 1 2 3 4 5 6 7 8 9
0 1 2 3 4 5 6 7 8 9
0 1 2 3 4 5 6 7 8 9
0 1 2 3 4 5 6 7 8 9
0 1 2 3 4 5 6 7 8 9
0 1 2 3 4 5 6 7 8 9
```

Image classification

Input: Handwritten digits /  
Images,  
Output: Digit  
 $n \rightarrow$  up to  $10^9$   
 $d$  (e.g., number of pixels)  $\rightarrow 10^6$

“Large scale” learning framework: both the number of examples  $n$  and the number of explanatory variables  $d$  are large.

# Supervised Machine Learning

- ▶ Consider an input/output pair  $(X, Y) \in \mathcal{X} \times \mathcal{Y}$ , following some unknown distribution  $\rho$ .
- ▶  $\mathcal{Y} = \mathbb{R}$  (regression) or  $\{-1, 1\}$  (classification).
- ▶ Goal: find a function  $\theta : \mathcal{X} \rightarrow \mathbb{R}$ , such that  $\theta(X)$  is a good prediction for  $Y$ .
- ▶ Prediction as a linear function  $\langle \theta, \Phi(X) \rangle$  of features  $\Phi(X) \in \mathbb{R}^d$ .
- ▶ Consider a loss function  $\ell : \mathcal{Y} \times \mathbb{R} \rightarrow \mathbb{R}_+$ : squared loss, logistic loss, 0-1 loss, etc.
- ▶ Define the Generalization risk (a.k.a., generalization error, “true risk”) as

$$\mathcal{R}(\theta) := \mathbb{E}_{\rho} [\ell(Y, \langle \theta, \Phi(X) \rangle)].$$

# Empirical Risk minimization (I)

- ▶ **Data:**  $n$  observations  $(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}$ ,  $i = 1, \dots, n$ , i.i.d.
  - ▶  $n$  very large, up to  $10^9$
  - ▶ Computer vision:  $d = 10^4$  to  $10^6$
- ▶ Empirical risk (or training error):

$$\hat{\mathcal{R}}(\theta) = \frac{1}{n} \sum_{i=1}^n \ell(y_i, \langle \theta, \Phi(x_i) \rangle).$$

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

$$\min_{\theta \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^n \ell(y_i, \langle \theta, \Phi(x_i) \rangle) + \mu \Omega(\theta).$$

convex data fitting term + regularizer

## Empirical Risk minimization (II)

For example, least-squares regression:

$$\min_{\theta \in \mathbb{R}^d} \frac{1}{2n} \sum_{i=1}^n (y_i - \langle \theta, \Phi(x_i) \rangle)^2 + \mu \Omega(\theta),$$

and logistic regression:

$$\min_{\theta \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^n \log (1 + \exp(-y_i \langle \theta, \Phi(x_i) \rangle)) + \mu \Omega(\theta).$$

Two fundamental questions: (1) computing (2) analyzing  $\hat{\theta}$ .

### Take home

- ▶ Problem is formalized as a **(convex) optimization problem**.
- ▶ In the **large scale setting**, high dimensional problem and many examples.

# Stochastic algorithms for ERM

$$\min_{\theta \in \mathbb{R}^d} \left\{ \hat{\mathcal{R}}(\theta) = \frac{1}{n} \sum_{i=1}^n \ell(y_i, \langle \theta, \Phi(x_i) \rangle) \right\}.$$

1. High dimension  $d \implies$  **First order algorithms**

**Gradient Descent (GD) :**

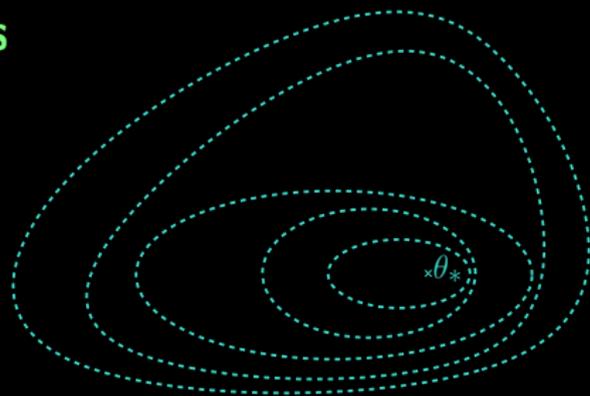
$$\theta_k = \theta_{k-1} - \gamma_k \hat{\mathcal{R}}'(\theta_{k-1})$$

Problem: computing the gradient costs  $O(dn)$  per iteration.

2. Large  $n \implies$  **Stochastic algorithms**

**Stochastic Gradient Descent (SGD)**

# Stochastic Gradient des



► Goal:

$$\min_{\theta \in \mathbb{R}^d} f(\theta)$$

given unbiased gradient estimates  $f'_n$

►  $\theta_* := \operatorname{argmin}_{\mathbb{R}^d} f(\theta)$ .



## SGD for ERM: $f = \hat{\mathcal{R}}$

Loss for a single pair of observations, for any  $j \leq n$ :

$$f_j(\theta) := \ell(y_j, \langle \theta, \Phi(x_j) \rangle).$$

One observation at each step  $\implies$  complexity  $O(d)$  per iteration.

For the **empirical risk**  $\hat{\mathcal{R}}(\theta) = \frac{1}{n} \sum_{k=1}^n \ell(y_k, \langle \theta, \Phi(x_k) \rangle)$ .

- ▶ At each step  $k \in \mathbb{N}^*$ , sample  $I_k \sim \mathcal{U}\{1, \dots, n\}$ , and use:

$$f'_{I_k}(\theta_{k-1}) = \ell'(y_{I_k}, \langle \theta_{k-1}, \Phi(x_{I_k}) \rangle)$$

- ▶ with  $\mathcal{F}_k = \sigma((x_i, y_i)_{1 \leq i \leq n}, (I_i)_{1 \leq i \leq k})$ ,

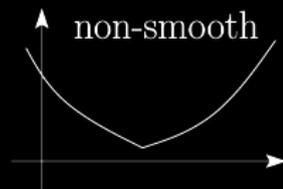
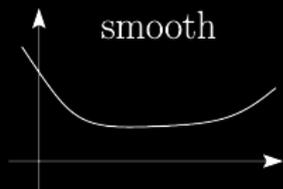
$$\mathbb{E}[f'_{I_k}(\theta_{k-1}) | \mathcal{F}_{k-1}] = \frac{1}{n} \sum_{k=1}^n \ell'(y_k, \langle \theta, \Phi(x_k) \rangle) = \hat{\mathcal{R}}'(\theta_{k-1}).$$

Mathematical framework: smoothness and/or strong convexity.

## Mathematical framework: Smoothness

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

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



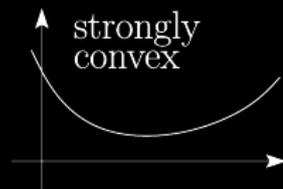
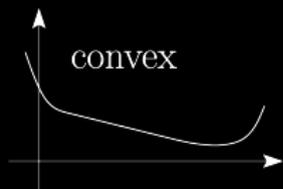
For all  $\theta \in \mathbb{R}^d$ :

$$g(\theta) \leq g(\theta') + \langle g'(\theta'), \theta - \theta' \rangle + L \|\theta - \theta'\|^2$$

# Mathematical framework: Strong Convexity

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

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



For all  $\theta \in \mathbb{R}^d$ :

$$g(\theta) \geq g(\theta') + \langle g'(\theta'), \theta - \theta' \rangle + \mu \|\theta - \theta'\|^2$$

## Application to machine learning

- ▶ We consider an a.s. convex loss in  $\theta$ . Thus  $\hat{\mathcal{R}}$  and  $\mathcal{R}$  are convex.
- ▶ Hessian of  $\hat{\mathcal{R}} \approx$  covariance matrix  $\frac{1}{n} \sum_{i=1}^n \Phi(x_i)\Phi(x_i)^\top$  ( $\simeq \mathbb{E}[\Phi(\mathbf{X})\Phi(\mathbf{X})^\top]$ .)

$$\hat{\mathcal{R}}''(\theta) = \frac{1}{n} \sum_{i=1}^n \left( \ell''(\langle \theta, \Phi(\mathbf{X}_i) \rangle, Y_i) \Phi(x_i)\Phi(x_i)^\top \right)$$

- ▶ If  $\ell$  is smooth, and  $\mathbb{E}[\|\Phi(\mathbf{X})\|^2] \leq r^2$ ,  $\mathcal{R}$  is smooth.
- ▶ If  $\ell$  is  $\mu$ -strongly convex, and **data has an invertible covariance matrix** (low correlation/dimension),  $\mathcal{R}$  is strongly convex.

## Analysis: behaviour of $(\theta_n)_{n \geq 0}$

$$\theta_k = \theta_{k-1} - \gamma_k f'_k(\theta_{k-1})$$

Importance of the **learning rate** (or sequence of step sizes)  $(\gamma_k)_{k \geq 0}$ . For smooth and strongly convex problem, traditional analysis shows Fabian (1968); Robbins and Siegmund (1985) that  $\theta_k \rightarrow \theta_*$  almost surely if

$$\sum_{k=1}^{\infty} \gamma_k = \infty \qquad \sum_{k=1}^{\infty} \gamma_k^2 < \infty.$$

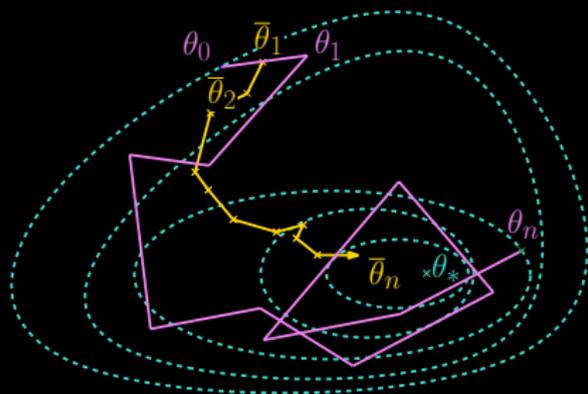
And asymptotic normality  $\sqrt{k}(\theta_k - \theta_*) \xrightarrow{d} \mathcal{N}(0, V)$ , for  $\gamma_k = \frac{\gamma_0}{k}$ ,  $\gamma_0 \geq \frac{1}{\mu}$ .

- ▶ Limit variance scales as  $1/\mu^2$
- ▶ Very sensitive to ill-conditioned problems.
- ▶  $\mu$  generally unknown, so hard to choose the step size...

# Polyak Ruppert averaging

Introduced by Polyak and Juditsky (1992) and Ruppert (1988):

$$\bar{\theta}_k = \frac{1}{k+1} \sum_{i=0}^k \theta_i.$$



- ▶ off line averaging reduces the noise effect.
- ▶ on line computing:  $\bar{\theta}_{k+1} = \frac{1}{k+1} \theta_{k+1} + \frac{k}{k+1} \bar{\theta}_k$ .
- ▶ one could also consider other averaging schemes (e.g., [Lecote, Juditsky et al. \(2012\)](#))

# Convex stochastic approximation: convergence

- ▶ Known **global** minimax rates of convergence for **non-smooth** problems Nemirovsky and Yudin (1983); Agarwal et al. (2012)
  - ▶ **Strongly convex**:  $O((\mu k)^{-1})$   
Attained by averaged stochastic gradient descent with  $\gamma_k \propto (\mu k)^{-1}$
  - ▶ **Non-strongly convex**:  $O(k^{-1/2})$   
Attained by averaged stochastic gradient descent with  $\gamma_k \propto k^{-1/2}$
- ▶ **Smooth** strongly convex problems
  - ▶ Rate  $\frac{1}{\mu k}$  for  $\gamma_k \propto k^{-1/2}$ : adapts to strong convexity.

Convergence rate for  $f(\tilde{\theta}_k) - f(\theta_*)$ , smooth  $f$ .

	min $\hat{\mathcal{R}}$	
	SGD	GD
Convex	$O\left(\frac{1}{\sqrt{k}}\right)$	$O\left(\frac{1}{k}\right)$
Stgly-Cvx	$O\left(\frac{1}{\mu k}\right)$	$O(e^{-\mu k})$

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⊖ Gradient descent update costs  $n$  times as much as SGD update.

Can we get best of both worlds ?

## Methods for finite sum minimization

- ▶ GD: at step  $k$ , use  $\frac{1}{n} \sum_{i=0}^n f'_i(\theta_k)$
- ▶ SGD: at step  $k$ , sample  $i_k \sim \mathcal{U}[1; n]$ , use  $f'_{i_k}(\theta_k)$
- ▶ SAG: at step  $k$ ,
  - ▶ keep a “full gradient”  $\frac{1}{n} \sum_{i=0}^n f'_i(\theta_{k_i})$ , with  $\theta_{k_i} \in \{\theta_1, \dots, \theta_k\}$
  - ▶ sample  $i_k \sim \mathcal{U}[1; n]$ , use

$$\frac{1}{n} \left( \sum_{i=0}^n f'_i(\theta_{k_i}) - f'_{i_k}(\theta_{k_{i_k}}) + f'_{i_k}(\theta_k) \right),$$

↷ ⊕ update costs the same as SGD

↷ ⊖ needs to store all gradients  $f'_i(\theta_{k_i})$  at “points in the past”

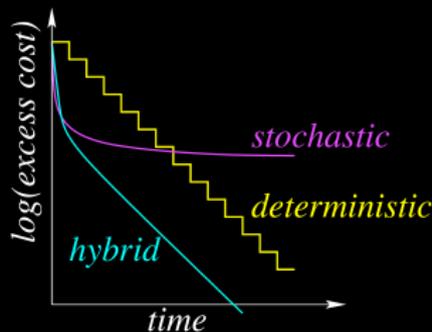
Some references:

- ▶ SAG Schmidt et al. (2013), SAGA Defazio et al. (2014a)
- ▶ SVRG Johnson and Zhang (2013) (reduces memory cost but 2 epochs...)
- ▶ FINITO Defazio et al. (2014b)
- ▶ S2GD Konečný and Richtárik (2013)...

And many others... See for example [Niao He's lecture notes](#) for a nice overview.

# Convergence rate for $f(\tilde{\theta}_k) - f(\theta_*)$ , smooth objective $f$ .

	$\min \hat{\mathcal{R}}$		
	SGD	GD	SAG
Convex	$O\left(\frac{1}{\sqrt{k}}\right)$	$O\left(\frac{1}{k}\right)$	
Stgly-Cvx	$O\left(\frac{1}{\mu k}\right)$	$O(e^{-\mu k})$	$O\left(1 - \left(\mu \wedge \frac{1}{n}\right)\right)^k$



GD, SGD, SAG (Fig. from Schmidt et al. (2013))

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Lower Bounds	$\alpha$	$\beta$	$\gamma$

$\alpha$  : Stoch. opt. information theoretic lower bounds, Agarwal et al. (2012);

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	SGD	AGD	SAG
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Stgly-Cvx	$O\left(\frac{1}{\mu k}\right)$	$O(e^{-\sqrt{\mu}k})$	$O\left(1 - (\mu \wedge \frac{1}{n})\right)^k$
Lower Bounds	$\alpha$	$\beta$	$\gamma$

$\alpha$ : Stoch. opt. information theoretic lower bounds, Agarwal et al. (2012);

$\beta$ : Black box first order optimization, Nesterov (2004);

$\gamma$ : Lower bounds for optimizing finite sums, Agarwal and Bottou (2014).

## Take home

### Stochastic algorithms for Empirical Risk Minimization.

- ▶ **Several algorithms** to optimize empirical risk, most efficient ones are **stochastic** and rely on **finite sum structure**
- ▶ **Stochastic algorithms** to optimize a **deterministic function**.
- ▶ Rates depend on the **regularity of the function**.

# What about generalization risk

Generalization guarantees:

- ▶ Uniform upper bound  $\sup_{\theta} \left| \hat{\mathcal{R}}(\theta) - \mathcal{R}(\theta) \right|$ . (empirical process theory)
- ▶ More precise: localized complexities (Bartlett et al., 2002), stability (Bousquet and Elisseeff, 2002).

Problems for ERM:

- ▶ Choose regularization (overfitting risk)
- ▶ How many iterations (i.e., passes on the data)?
- ▶ Generalization guarantees generally of order  $O(1/\sqrt{n})$ , no need to be precise

2 important insights:

1. No need to optimize below statistical error,
2. Generalization risk is more important than empirical risk.

**SGD can be used to minimize the generalization risk.**

## SGD for the generalization risk: $f = \mathcal{R}$

SGD: key assumption  $\mathbb{E}[f'_n(\theta_{n-1}) | \mathcal{F}_{n-1}] = f'(\theta_{n-1})$ .

For the **risk**

$$\mathcal{R}(\theta) = \mathbb{E}_\rho [\ell(Y, \langle \theta, \Phi(X) \rangle)]$$

- ▶ At step  $0 < k \leq n$ , use a new point independent of  $\theta_{k-1}$ :

$$f'_k(\theta_{k-1}) = \ell'(y_k, \langle \theta_{k-1}, \Phi(x_k) \rangle)$$

- ▶ For  $0 \leq k \leq n$ ,  $\mathcal{F}_k = \sigma((x_i, y_i)_{1 \leq i \leq k})$ .

$$\begin{aligned} \mathbb{E}[f'_k(\theta_{k-1}) | \mathcal{F}_{k-1}] &= \mathbb{E}_\rho[\ell'(y_k, \langle \theta_{k-1}, \Phi(x_k) \rangle) | \mathcal{F}_{k-1}] \\ &= \mathbb{E}_\rho[\ell'(Y, \langle \theta_{k-1}, \Phi(X) \rangle)] = \mathcal{R}'(\theta_{k-1}) \end{aligned}$$

- ▶ Single pass through the data, Running-time =  $O(nd)$ ,
- ▶ “Automatic” regularization.

# SGD for the generalization risk: $f = \mathcal{R}$

ERM minimization

several passes :  $0 \leq k$

$x_i, y_i$  is  $\mathcal{F}_t$ -measurable for any  $t$

Gen. risk minimization

One pass  $0 \leq k \leq n$

$\mathcal{F}_t$ -measurable for  $t \geq i$ .

# Convergence rate for $f(\tilde{\theta}_k) - f(\theta_*)$ , smooth objective $f$ .

	min $\hat{\mathcal{R}}$			min $\mathcal{R}$
	SGD	GD	SAG	SGD
Convex	$O\left(\frac{1}{\sqrt{k}}\right)$	$O\left(\frac{1}{k}\right)$		$O\left(\frac{1}{\sqrt{k}}\right)$
Stgly-Cvx	$O\left(\frac{1}{\mu k}\right)$	$O(e^{-\mu k})$	$O\left(1 - \left(\mu \wedge \frac{1}{n}\right)\right)^k$	$O\left(\frac{1}{\mu k}\right)$

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Lower Bounds	$\alpha$	$\beta$	$\gamma$	$\delta$
		$0 \leq k$		$0 \leq k \leq n$

$\delta$  : Information theoretic LB - Statistical theory (Tsybakov, 2003).

Gradient is unknown

## Least Mean Squares: rate independent of $\mu$

- ▶ Least-squares:  $\mathcal{R}(\theta) = \frac{1}{2}\mathbb{E}[(Y - \langle \Phi(X), \theta \rangle)^2]$  with  $\theta \in \mathbb{R}^d$ 
  - ▶ SGD = least-mean-square algorithm
  - ▶ Usually studied without averaging and decreasing step-sizes.
- ▶ New analysis for averaging and constant step-size  $\gamma = 1/(4R^2)$  Bach and Moulines (2013)
  - ▶ Assume  $\|\Phi(x_n)\| \leq r$  and  $|y_n - \langle \Phi(x_n), \theta_* \rangle| \leq \sigma$  almost surely
  - ▶ No assumption regarding lowest eigenvalues of the Hessian
  - ▶ Main result:

$$\mathbb{E}\mathcal{R}(\bar{\theta}_n) - \mathcal{R}(\theta_*) \leq \frac{4\sigma^2 d}{n} + \frac{\|\theta_0 - \theta_*\|^2}{\gamma n}$$

- ▶ Matches statistical lower bound (Tsybakov, 2003).
- ▶ Optimal rate with “large” (constant) step sizes

## Take home

- ▶ SGD can be used to minimize the true risk directly
- ▶ **Stochastic algorithm to minimize unknown function**
- ▶ No regularization needed, only one pass
- ▶ For Least Squares, with constant step, optimal rate .

## Take home

- ▶ SGD can be used to minimize the true risk directly
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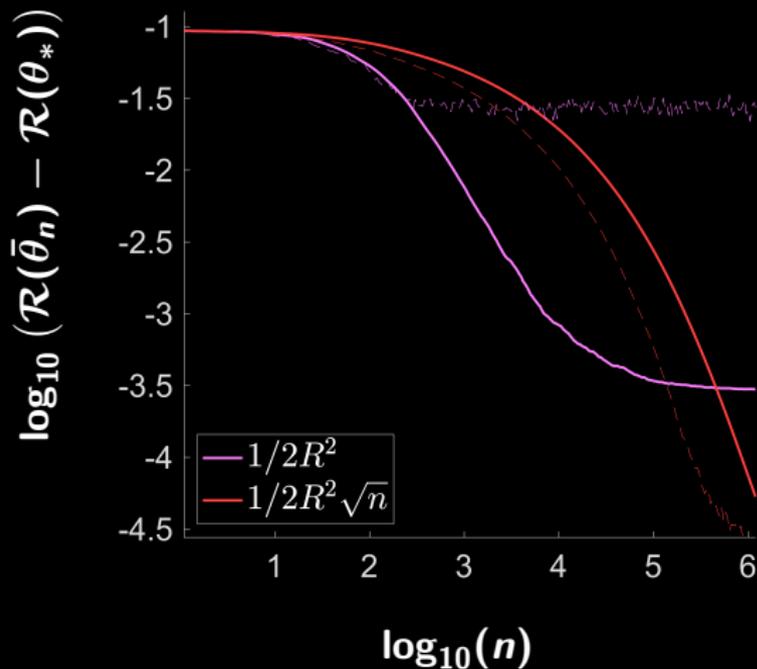
↪ **Stochastic approximation, beyond Least Squares ?**

## Beyond finite dimensional Least squares

- ▶ Beyond parametric models: Non Parametric Stochastic Approximation with Large step sizes. (Dieuleveut and Bach, 2015)
- ▶ Improved Sampling: Averaged least-mean-squares: bias-variance trade-offs and optimal sampling distributions. (Défossez and Bach, 2015)
- ▶ Acceleration: Harder, Better, Faster, Stronger Convergence Rates for Least-Squares Regression. (Dieuleveut et al., 2016)
- ▶ Beyond smoothness and euclidean geometry: Stochastic Composite Least-Squares Regression with convergence rate  $O(1/n)$ . (Flammarion and Bach, 2017)
- ▶ **General smooth and strongly convex optimization: Bridging the Gap between Constant Step Size Stochastic Gradient Descent and Markov Chains (Dieuleveut et al., 2017).**

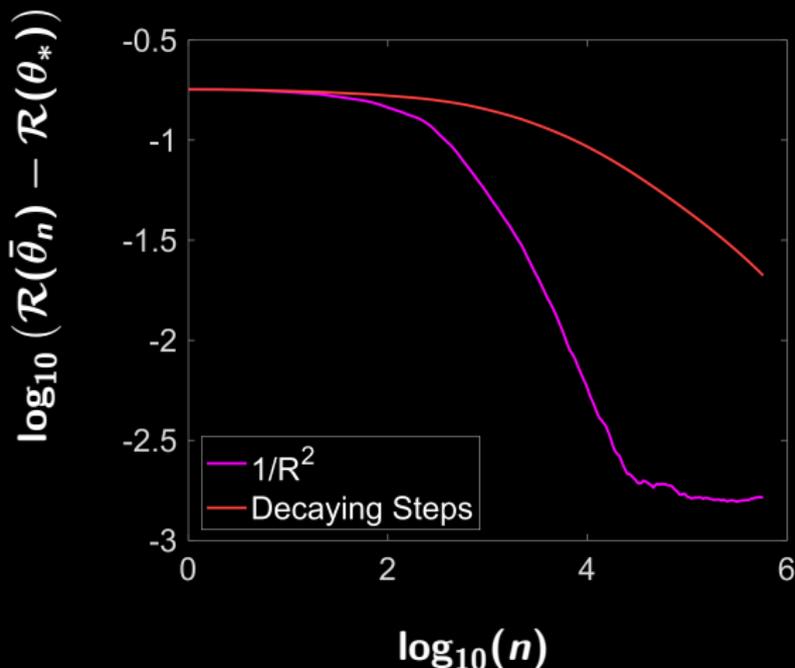
## Beyond least squares. Logistic regression

$$\min_{\theta \in \mathbb{D}^d} \mathbb{E} \log \left( 1 + \exp(-Y \langle \theta, \Phi(X) \rangle) \right).$$



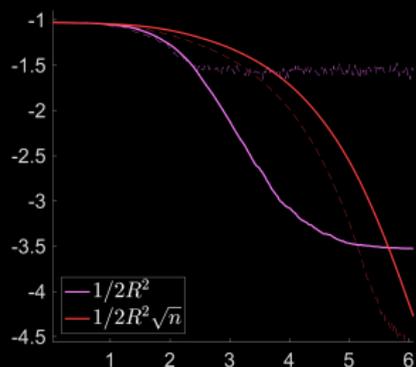
Logistic regression. Final iterate (dashed), and averaged recursion (plain).

# Beyond least squares. Logistic regression, real data



Logistic regression, Covertypе dataset,  $n = 581012$ ,  $d = 54$ .  
Comparison between a constant learning rate and decaying  
learning rate as  $\frac{1}{\sqrt{n}}$ .

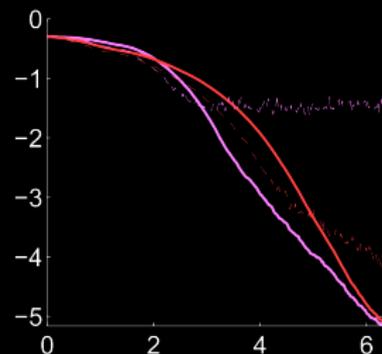
## Motivation 2/ 2. Difference between quadratic and logistic loss



**Logistic Regression**

$$\mathbb{E}\mathcal{R}(\bar{\theta}_n) - \mathcal{R}(\theta_*) = O(\gamma^2)$$

$$\text{with } \gamma = 1/(4R^2)$$



**Least-Squares Regression**

$$\mathbb{E}\mathcal{R}(\bar{\theta}_n) - \mathcal{R}(\theta_*) = O\left(\frac{1}{n}\right)$$

$$\text{with } \gamma = 1/(4R^2)$$

# SGD: an homogeneous Markov chain

Consider a  $L$ -smooth and  $\mu$ -strongly convex function  $\mathcal{R}$ .

SGD with a step-size  $\gamma > 0$  is an **homogeneous Markov chain**:

$$\theta_{k+1}^\gamma = \theta_k^\gamma - \gamma [\mathcal{R}'(\theta_k^\gamma) + \varepsilon_{k+1}(\theta_k^\gamma)] ,$$

- ▶ satisfies Markov property
- ▶ is homogeneous, for  $\gamma$  constant,  $(\varepsilon_k)_{k \in \mathbb{N}}$  i.i.d.

Also assume:

- ▶  $\mathcal{R}'_k = \mathcal{R}' + \varepsilon_{k+1}$  is almost surely  $L$ -co-coercive.
- ▶ Bounded moments

$$\mathbb{E}[\|\varepsilon_k(\theta_*)\|^4] < \infty.$$

# Stochastic gradient descent as a Markov Chain: Analysis framework<sup>†</sup>

- ▶ Existence of a limit distribution  $\pi_\gamma$ , and linear convergence to this distribution:

$$\theta_k^\gamma \xrightarrow{d} \pi_\gamma.$$

- ▶ Convergence of second order moments of the chain,

$$\bar{\theta}_k^\gamma \xrightarrow[k \rightarrow \infty]{L^2} \bar{\theta}_\gamma := \mathbb{E}_{\pi_\gamma} [\theta].$$

- ▶ Behavior under the limit distribution ( $\gamma \rightarrow 0$ ):  $\bar{\theta}_\gamma = \theta_* + ?$ .

↪ Provable convergence improvement with extrapolation tricks.

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<sup>†</sup>Dieuleveut, Durmus, Bach [2017].

# Existence of a limit distribution $\gamma \rightarrow 0$

Goal:

$$(\theta_k^\gamma)_{k \geq 0} \xrightarrow{d} \pi_\gamma .$$

## Theorem

For any  $\gamma < L^{-1}$ , the chain  $(\theta_k^\gamma)_{k \geq 0}$  admits a unique stationary distribution  $\pi_\gamma$ . In addition for all  $\theta_0 \in \mathbb{R}^d$ ,  $k \in \mathbb{N}$ :

$$W_2^2(\theta_k^\gamma, \pi_\gamma) \leq (1 - 2\mu\gamma(1 - \gamma L))^k \int_{\mathbb{R}^d} \|\theta_0 - \vartheta\|^2 d\pi_\gamma(\vartheta) .$$

**Wasserstein metric:** distance between probability measures.

## Behavior under limit distribution.

Ergodic theorem:  $\bar{\theta}_k \rightarrow \mathbb{E}_{\pi_\gamma}[\theta] =: \bar{\theta}_\gamma$ . Where is  $\bar{\theta}_\gamma$  ?

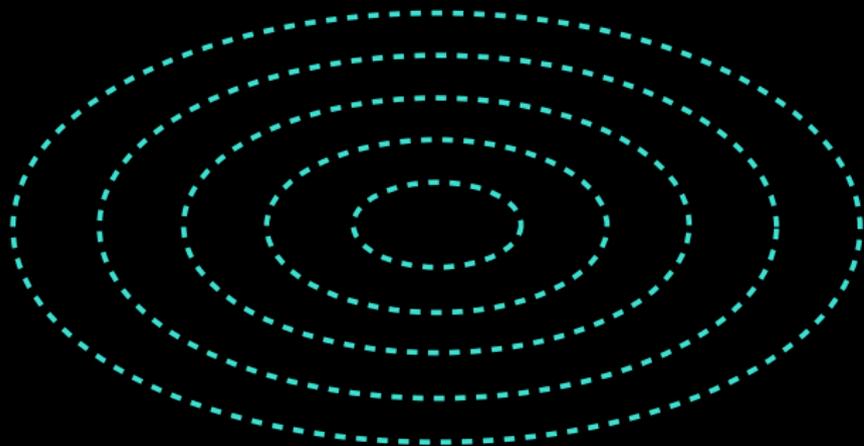
If  $\theta_0 \sim \pi_\gamma$ , then  $\theta_1 \sim \pi_\gamma$ .

$$\theta_1^\gamma = \theta_0^\gamma - \gamma[\mathcal{R}'(\theta_0^\gamma) + \varepsilon_1(\theta_0^\gamma)] .$$

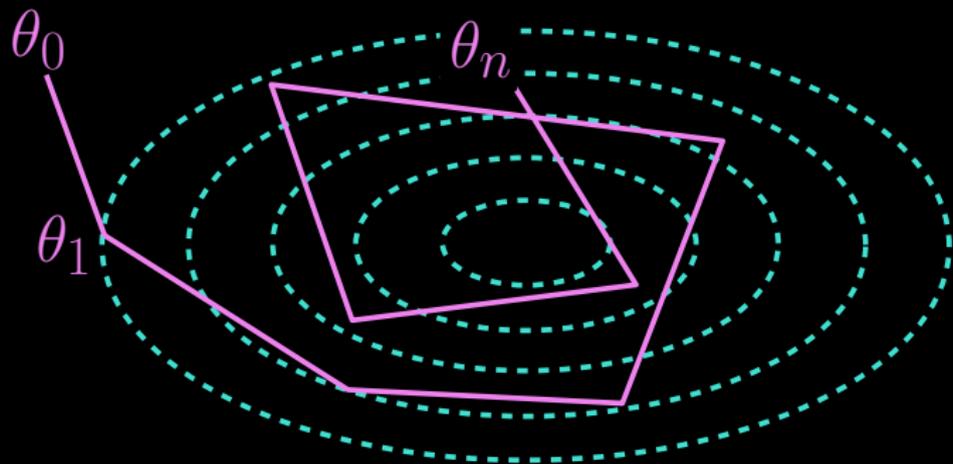
$$\mathbb{E}_{\pi_\gamma} [\mathcal{R}'(\theta)] = 0$$

In the **quadratic case** (linear gradients)  $\Sigma \mathbb{E}_{\pi_\gamma} [\theta - \theta_*] = 0$ :  $\bar{\theta}_\gamma = \theta_*$ !

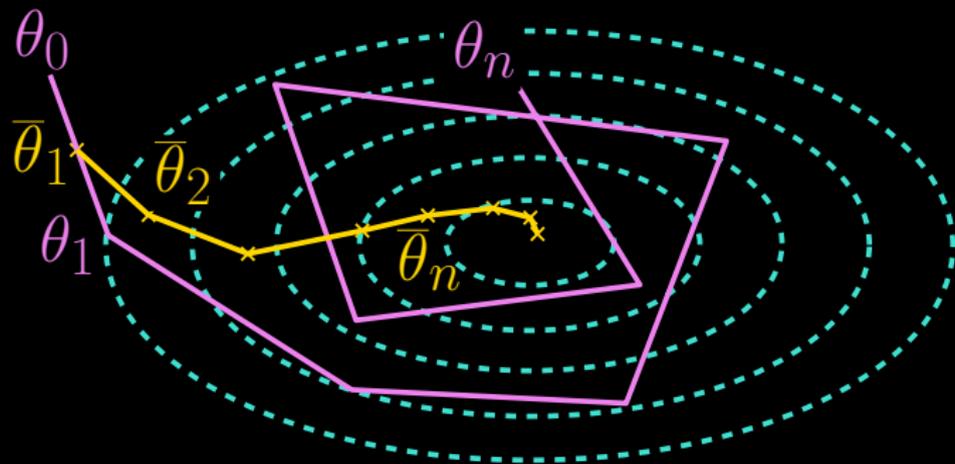
# Constant learning rate SGD: convergence in the quadratic case



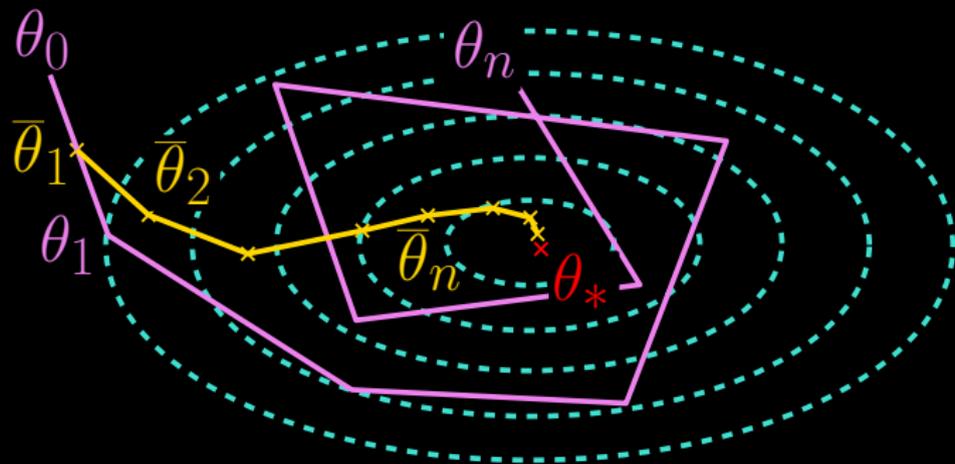
## Constant learning rate SGD: convergence in the quadratic case



# Constant learning rate SGD: convergence in the quadratic case



# Constant learning rate SGD: convergence in the quadratic case



## Behavior under limit distribution.

Ergodic theorem:  $\bar{\theta}_n \rightarrow \mathbb{E}_{\pi_\gamma}[\theta] =: \bar{\theta}_\gamma$ . Where is  $\bar{\theta}_\gamma$  ?

If  $\theta_0 \sim \pi_\gamma$ , then  $\theta_1 \sim \pi_\gamma$ .

$$\theta_1^\gamma = \theta_0^\gamma - \gamma [\mathcal{R}'(\theta_0^\gamma) + \varepsilon_1(\theta_0^\gamma)] .$$

$$\mathbb{E}_{\pi_\gamma} [\mathcal{R}'(\theta)] = 0$$

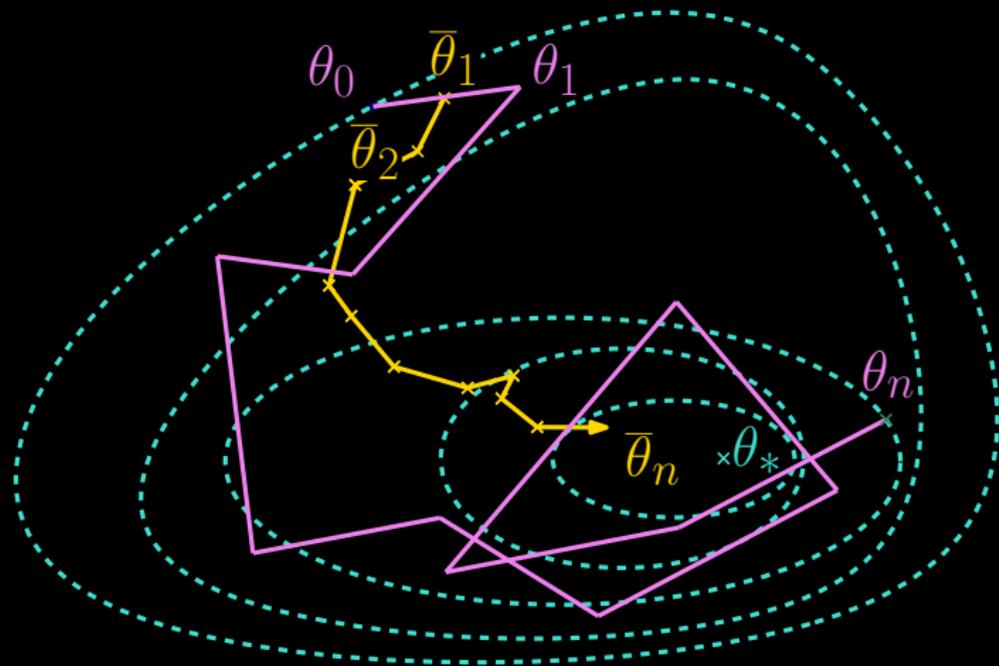
In the **quadratic case** (linear gradients)  $\Sigma \mathbb{E}_{\pi_\gamma} [\theta - \theta_*] = 0$ :  $\bar{\theta}_\gamma = \theta_*$ !

In the **general case**, Taylor expansion of  $\mathcal{R}$ , and same reasoning on higher moments of the chain leads to

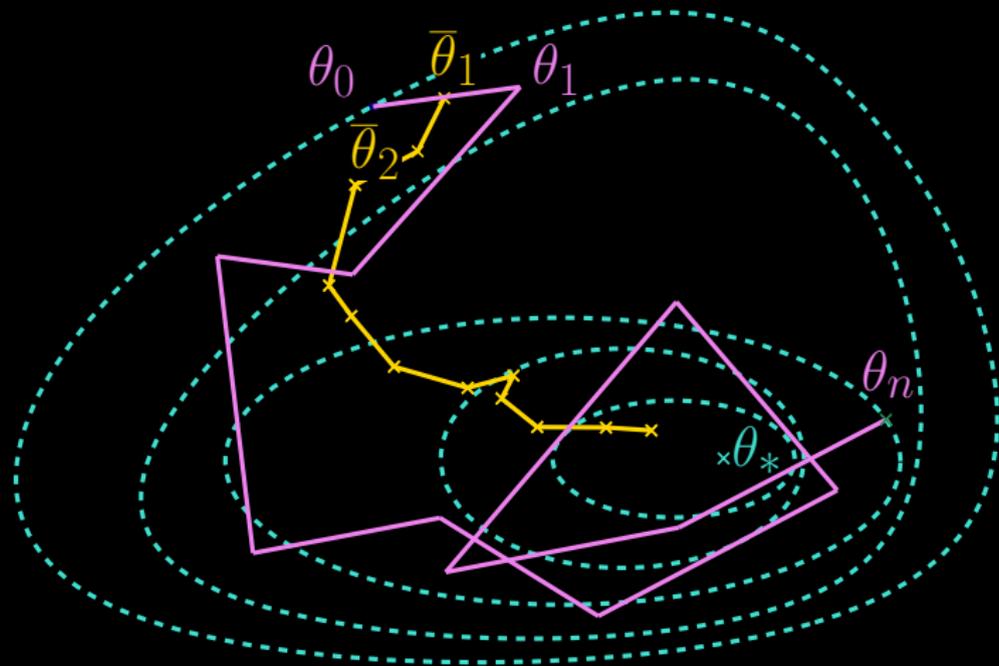
$$\bar{\theta}_\gamma - \theta_* \simeq \gamma \mathcal{R}''(\theta_*)^{-1} \mathcal{R}'''(\theta_*) \left( [\mathcal{R}''(\theta_*) \otimes I + I \otimes \mathcal{R}''(\theta_*)]^{-1} \mathbb{E}_\varepsilon[\varepsilon(\theta_*)^{\otimes 2}] \right)$$

$$\text{Overall, } \bar{\theta}_\gamma - \theta_* = \gamma \Delta + O(\gamma^2).$$

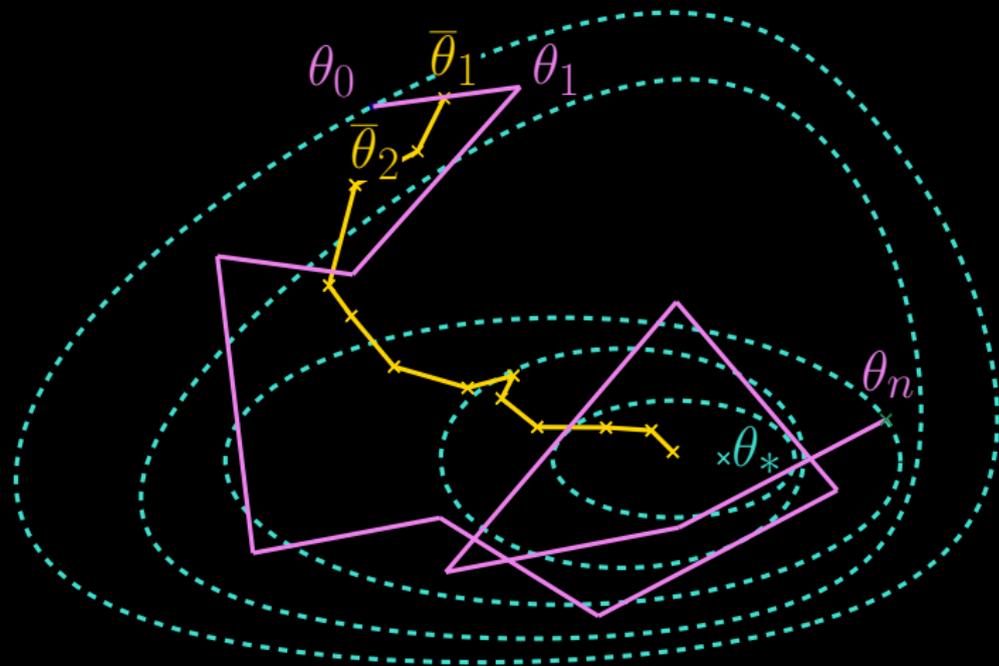
# Constant learning rate SGD: convergence in the non-quadratic case



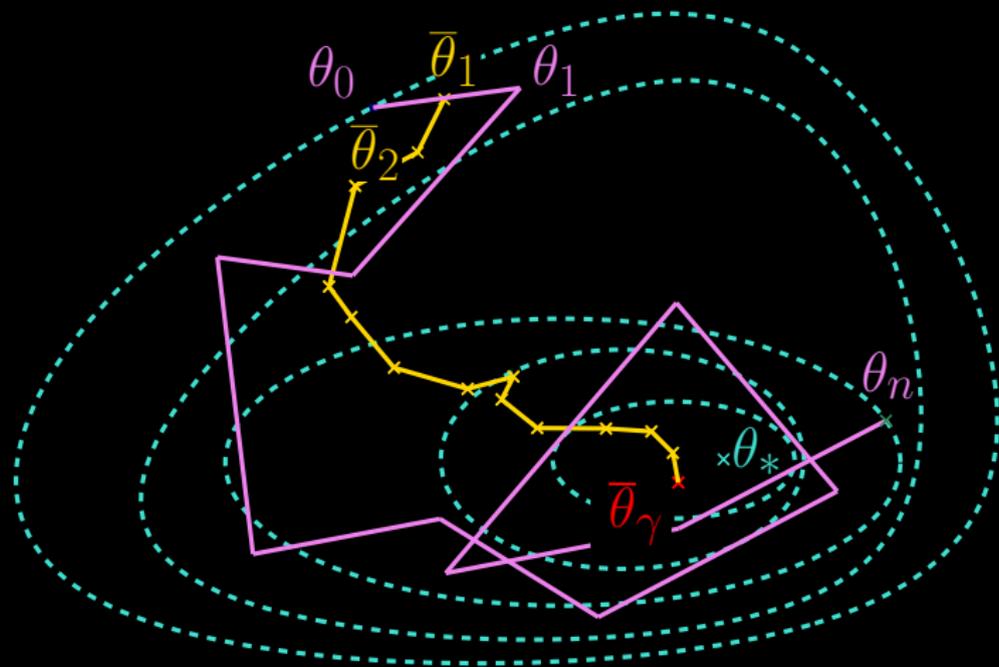
# Constant learning rate SGD: convergence in the non-quadratic case



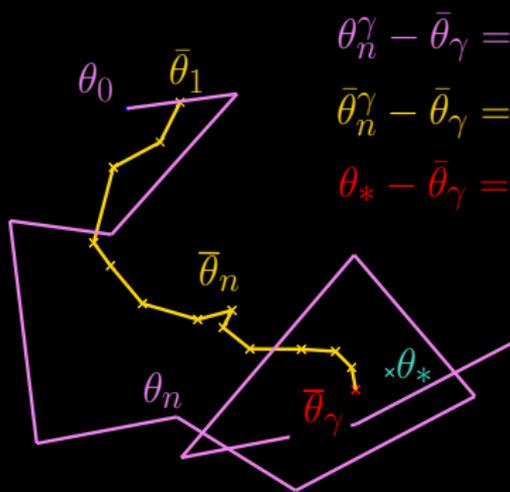
# Constant learning rate SGD: convergence in the non-quadratic case



# Constant learning rate SGD: convergence in the non-quadratic case



# Richardson extrapolation



$$\theta_n^\gamma - \bar{\theta}_\gamma = O_p(\gamma^{1/2})$$

$$\bar{\theta}_n^\gamma - \bar{\theta}_\gamma = O_p(n^{-1/2})$$

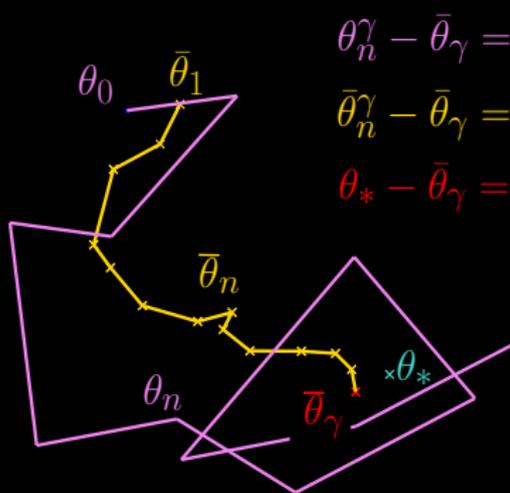
$$\theta_* - \bar{\theta}_\gamma = O(\gamma)$$

$\bullet \theta_*$

$\bullet \leftarrow \theta_* + \gamma \Delta$

Recovering convergence closer to  $\theta_*$  by Richardson extrapolation  $2\bar{\theta}_n^\gamma - \bar{\theta}_n^{2\gamma}$

# Richardson extrapolation



$$\theta_n^\gamma - \bar{\theta}_\gamma = O_p(\gamma^{1/2})$$

$$\bar{\theta}_n^\gamma - \bar{\theta}_\gamma = O_p(n^{-1/2})$$

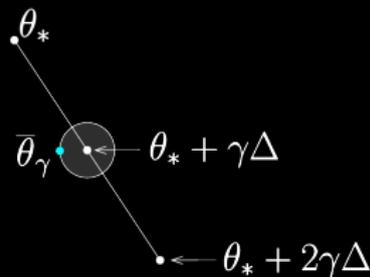
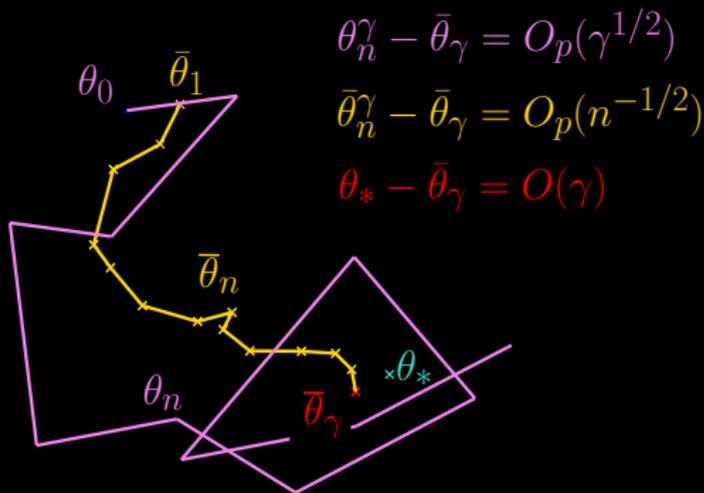
$$\theta_* - \bar{\theta}_\gamma = O(\gamma)$$

$\theta_*$

$$\bar{\theta}_\gamma \leftarrow \theta_* + \gamma \Delta$$

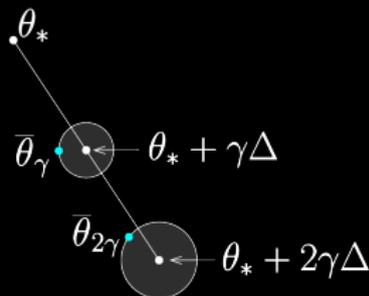
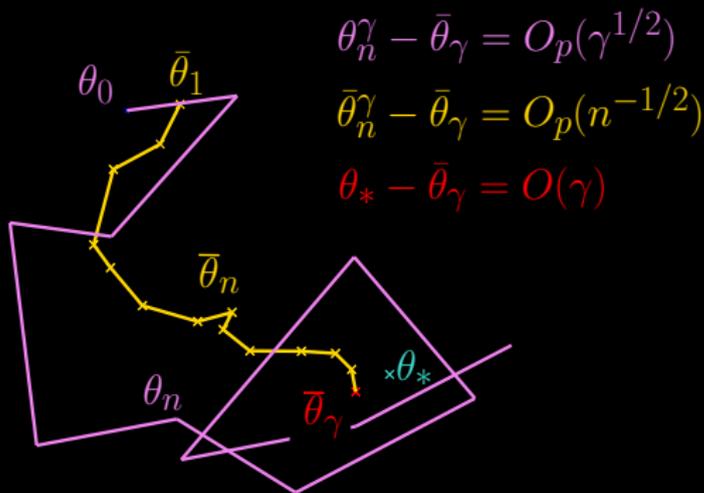
Recovering convergence closer to  $\theta_*$  by Richardson extrapolation  $2\bar{\theta}_n^\gamma - \bar{\theta}_n^{2\gamma}$

# Richardson extrapolation



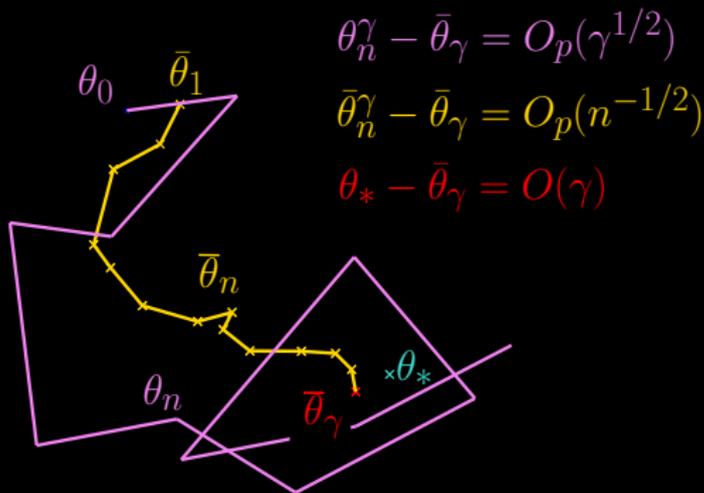
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# Richardson extrapolation



Recovering convergence closer to  $\theta_*$  by Richardson extrapolation  $2\bar{\theta}_n^\gamma - \bar{\theta}_n^{2\gamma}$

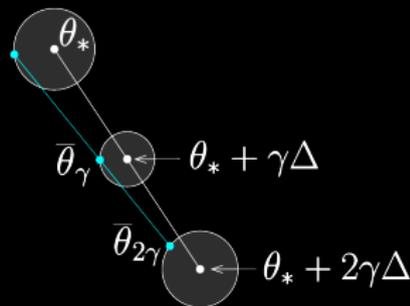
# Richardson extrapolation



$$\theta_n^\gamma - \bar{\theta}_\gamma = O_p(\gamma^{1/2})$$

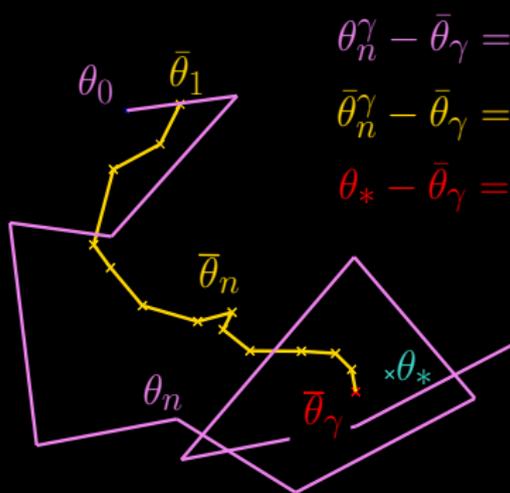
$$\bar{\theta}_n^\gamma - \bar{\theta}_\gamma = O_p(n^{-1/2})$$

$$\theta_* - \bar{\theta}_\gamma = O(\gamma)$$



Recovering convergence closer to  $\theta_*$  by Richardson extrapolation  $2\bar{\theta}_n^\gamma - \bar{\theta}_n^{2\gamma}$

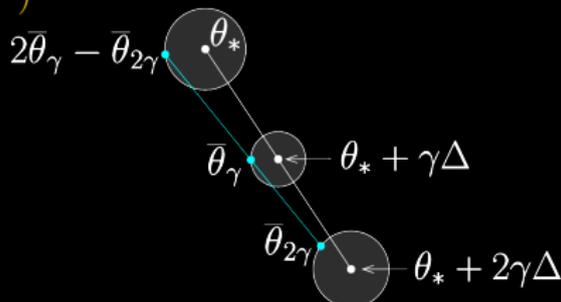
# Richardson extrapolation



$$\theta_n^\gamma - \bar{\theta}_\gamma = O_p(\gamma^{1/2})$$

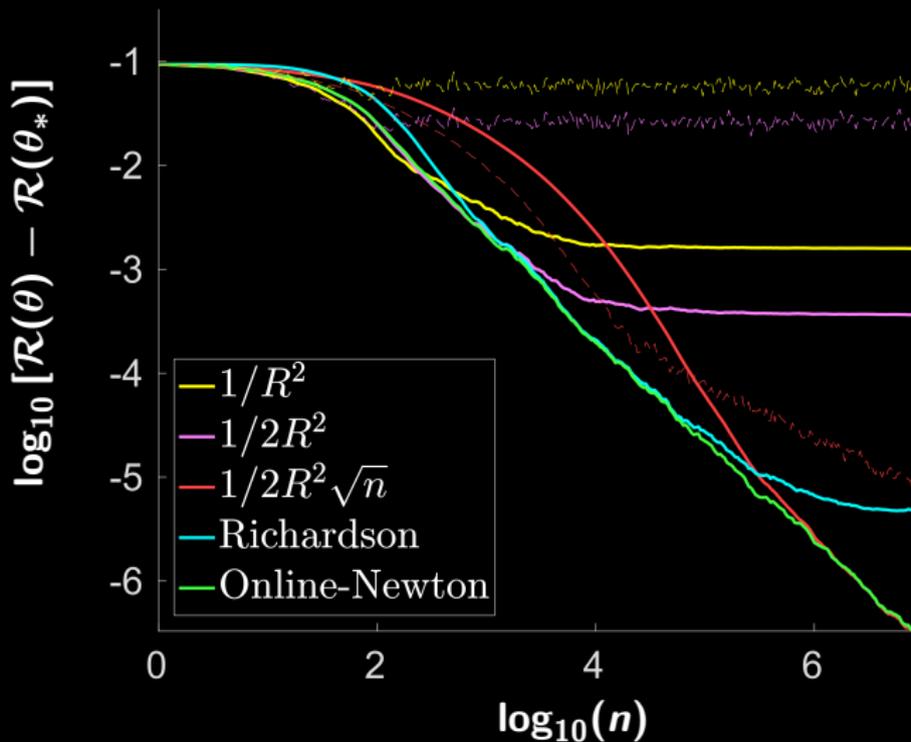
$$\bar{\theta}_n^\gamma - \bar{\theta}_\gamma = O_p(n^{-1/2})$$

$$\theta_* - \bar{\theta}_\gamma = O(\gamma)$$



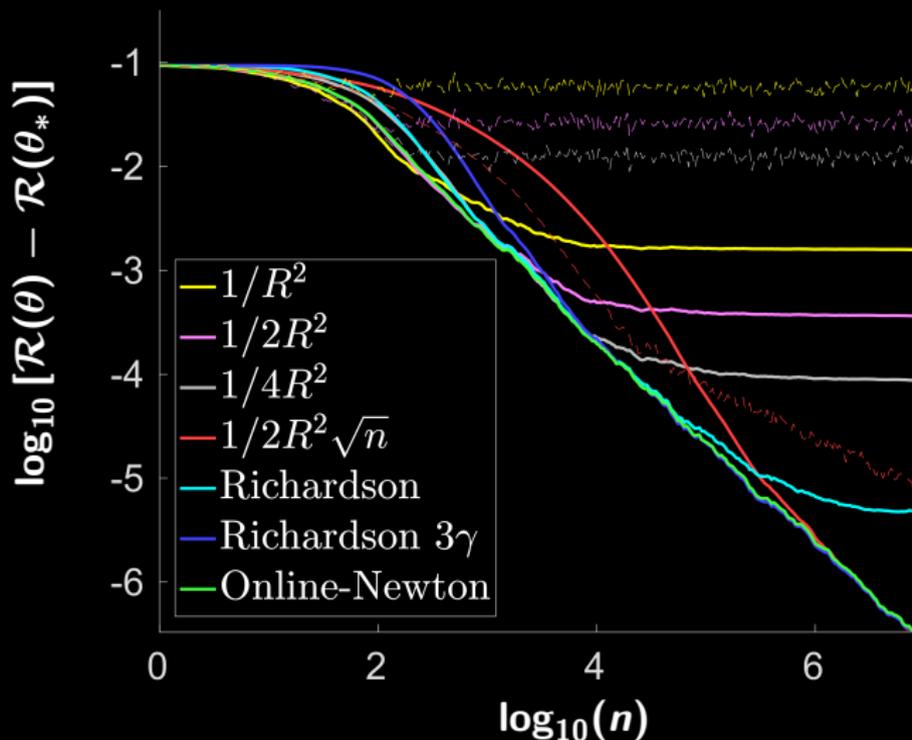
Recovering convergence closer to  $\theta_*$  by Richardson extrapolation  $2\bar{\theta}_n^\gamma - \bar{\theta}_n^{2\gamma}$

## Experiments: smaller dimension



Synthetic data, logistic regression,  $n = 8 \cdot 10^6$

# Experiments: Double Richardson



Synthetic data, logistic regression,  $n = 8.10^6$

“Richardson  $3\gamma$ ”: estimator built using Richardson on 3 different sequences:  $\tilde{\theta}_n^3 = \frac{8}{3}\bar{\theta}_n^\gamma - 2\bar{\theta}_n^{2\gamma} + \frac{1}{3}\bar{\theta}_n^{4\gamma}$

# Conclusion MC

## Take home

- ▶ Asymptotic sometimes matter less than first iterations: consider large step size.
- ▶ Constant step size SGD is a homogeneous Markov chain.
- ▶ Difference between LS and general smooth loss is intuitive.

## For smooth strongly convex loss:

- ▶ Convergence in terms of Wasserstein distance.
- ▶ Decomposition as three sources of error: variance, initial conditions, and “drift”
- ▶ Detailed analysis of the position of the limit point: the direction does not depend on  $\gamma$  at first order  $\implies$  Extrapolation tricks can help.

## Further references

Many stochastic algorithms not covered in this talk  
(coordinate descent, online Newton, composite optimization,  
non convex learning) ...

- ▶ Good introduction: [Francis's lecture notes at Orsay](#)
- ▶ Book: [Convex Optimization: Algorithms and Complexity,](#)  
Sébastien Bubeck

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