

Stochastic Algorithms in Machine Learning

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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: definition & applications

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
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 ρ .
- ▶ $\mathcal{Y} = \mathbb{R}$ (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

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

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 $\hat{\theta}$ and (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 descent

- **Goal:**

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

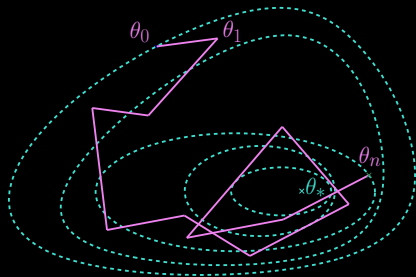
given unbiased gradient estimates f'_n

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

- **Key algorithm: Stochastic Gradient Descent (SGD)** (Robbins and Monro, 1951):

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

- $\mathbb{E}[f'_k(\theta_{k-1}) | \mathcal{F}_{k-1}] = f'(\theta_{k-1})$ for a filtration $(\mathcal{F}_k)_{k \geq 0}$, θ_k is \mathcal{F}_k measurable.



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

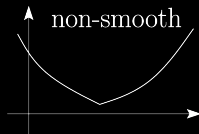
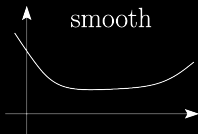
$$\mathbb{E}[f'_{I_k}(\theta_{k-1}) | \mathcal{F}_{k-1}] = \frac{1}{n} \sum_{k=1}^n \ell'(y_k, \langle \theta, \Phi(x_k) \rangle) = \hat{\mathcal{R}}'(\theta_{k-1}).$$

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

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



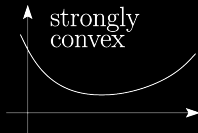
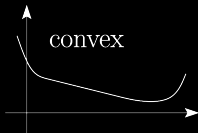
For all $\theta \in \mathbb{R}^d$:

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

Mathematical framework: Strong Convexity

- ▶ A twice differentiable function $g : \mathbb{R}^d \rightarrow \mathbb{R}$ is μ -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 θ . Thus $\hat{\mathcal{R}}$ and \mathcal{R} are convex.
- ▶ Hessian of $\hat{\mathcal{R}} \approx$ covariance matrix $\frac{1}{n} \sum_{i=1}^n \Phi(x_i)\Phi(x_i)^\top$ ($\simeq \mathbb{E}[\Phi(X)\Phi(X)^\top]$.)

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

- ▶ If ℓ is smooth, and $\mathbb{E}[\|\Phi(X)\|^2] \leq r^2$, \mathcal{R} is smooth.
- ▶ If ℓ is μ -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

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

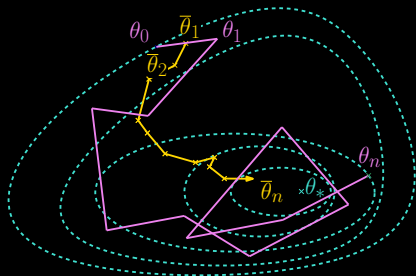
And asymptotic normality $\sqrt{k}(\theta_k - \theta_*) \xrightarrow{d} \mathcal{N}(0, V)$, for $\gamma_k = \frac{\gamma_0}{k}$, $\gamma_0 \geq \frac{1}{\mu}$.

- ▶ Limit variance scales as $1/\mu^2$
- ▶ Very sensitive to ill-conditioned problems.
- ▶ μ 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., Lacoste-Julien et al. (2012)).

Convex stochastic approximation: convergence results

- ▶ 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** objective f .

(all rates have hidden dependences in the smoothness)

	$\min \hat{\mathcal{R}}$	
	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

Key idea: using a random gradient with **less variance**.

- ▶ **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

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

↗ \oplus update costs the same as SGD

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

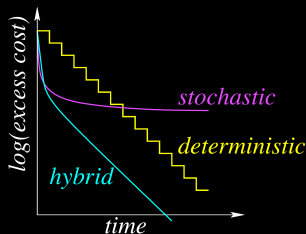
Some references:

- ▶ 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	$O\left(\frac{1}{\mu k}\right)$	$O(e^{-\mu k})$	$O\left(1 - (\mu \wedge \frac{1}{n})\right)^k$



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

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Lower Bounds	α	β	γ

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

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Lower Bounds	α	β	γ

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

β : Black box first order optimization, Nesterov (2004);

γ : 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 θ_{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.**

	ERM minimization	Gen. risk minimization
	several passes : $0 \leq k$	One pass $0 \leq k \leq n$
x_i, y_i is	\mathcal{F}_t -measurable for any t	\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	AGD	SAG	SGD	
Convex	$O\left(\frac{1}{\sqrt{k}}\right)$	$O\left(\frac{1}{k^2}\right)$		$O\left(\frac{1}{\sqrt{k}}\right)$	
Stgly-Cvx	$O\left(\frac{1}{\mu k}\right)$	$O(e^{-\sqrt{\mu}k})$	$O\left(1 - (\mu \wedge \frac{1}{n})\right)^k$	$O\left(\frac{1}{\mu k}\right)$	

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		$0 \leq k$		$0 \leq k \leq n$
Lower Bounds	α	β	γ	δ

δ : Information theoretic LB - Statistical theory (Tsybakov, 2003).

Gradient is unknown

Least Mean Squares: rate independent of μ

- ▶ **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 .

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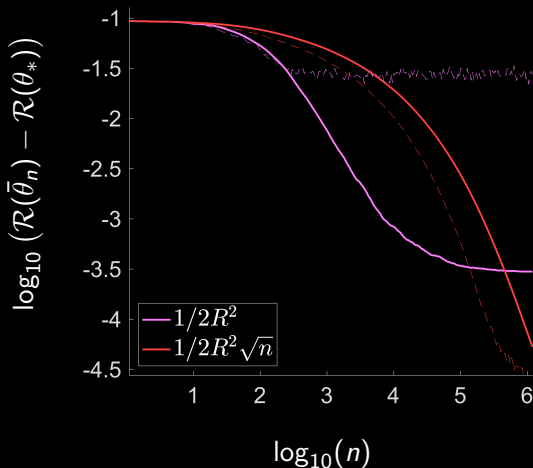
↪ Stochastic approximation, beyond Least Squares ?

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).

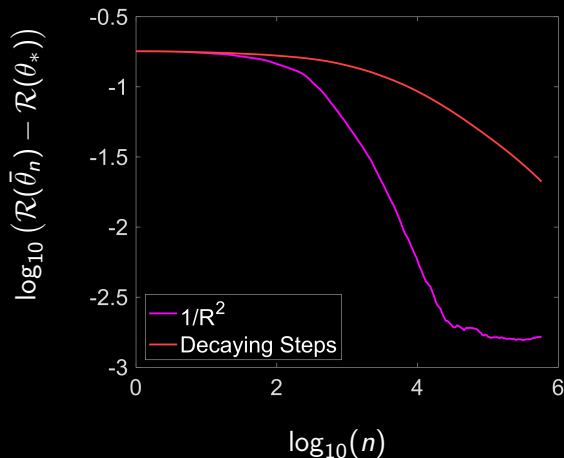
Beyond least squares. Logistic regression

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



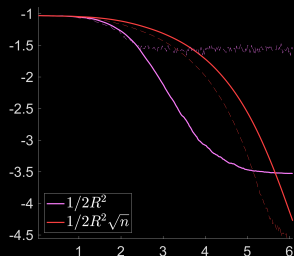
Logistic regression. Final iterate (dashed), and averaged recursion (plain).

Beyond least squares. Logistic regression, real data



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

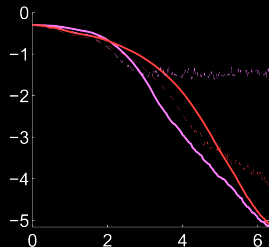
Motivation 2/ 2. Difference between quadratic and logistic loss



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 μ -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 γ 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[†]

- ▶ Existence of a limit distribution π_γ , 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.

[†]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 π_γ . 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 $\bar{\theta}_\gamma$?

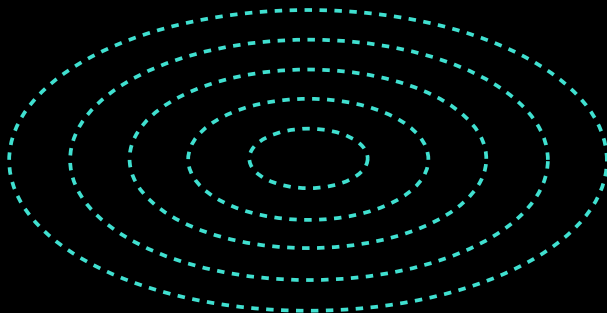
If $\theta_0 \sim \pi_\gamma$, then $\theta_1 \sim \pi_\gamma$.

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

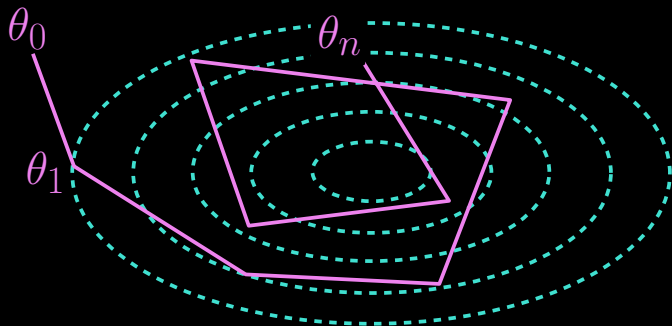
$$\mathbb{E}_{\pi_\gamma} [\mathcal{R}'(\theta)] = 0$$

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

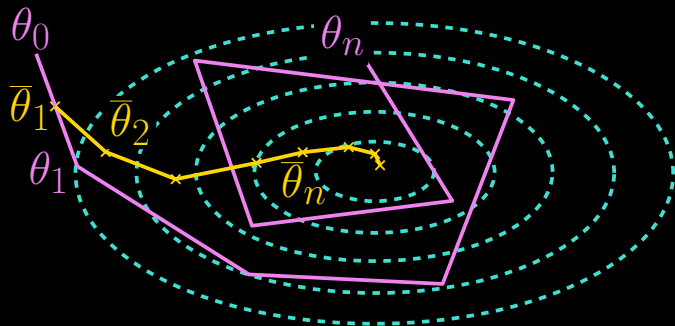
Constant learning rate SGD: convergence in the quadratic case



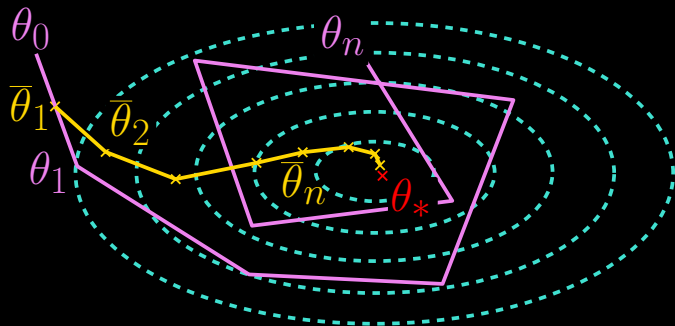
Constant learning rate SGD: convergence in the quadratic case



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 $\theta_1 \sim \pi_\gamma$.

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

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

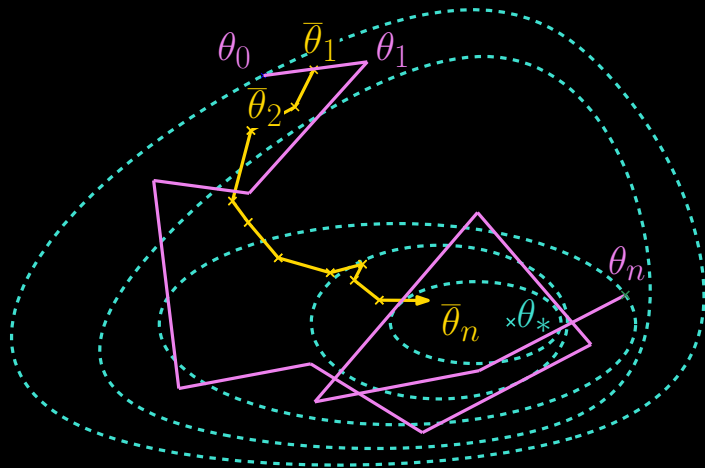
In the **quadratic case** (linear gradients) $\Sigma \mathbb{E}_{\pi_\gamma} [\theta - \theta_*] = 0$: $\bar{\theta}_\gamma = \theta_*$!

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

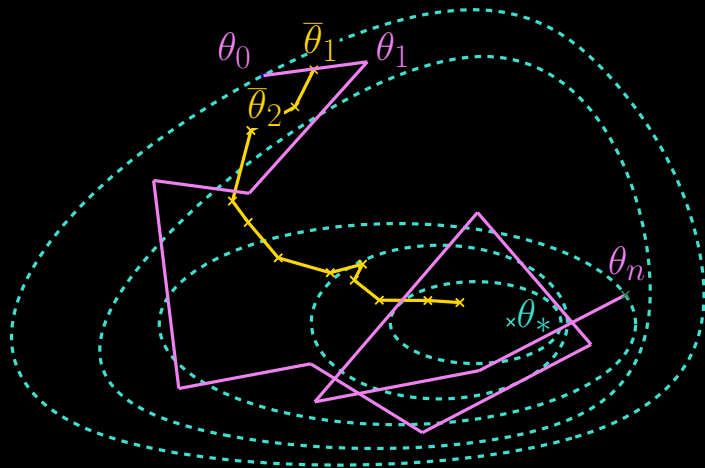
$$\bar{\theta}_\gamma - \theta_* = \gamma \mathcal{R}''(\theta_*)^{-1} \mathcal{R}'''(\theta_*) \left([\mathcal{R}''(\theta_*) \otimes I + I \otimes \mathcal{R}''(\theta_*)]^{-1} \mathbb{E}_\varepsilon [\varepsilon(\theta_*)^{\otimes 2}] \right) + O(\gamma^2)$$

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

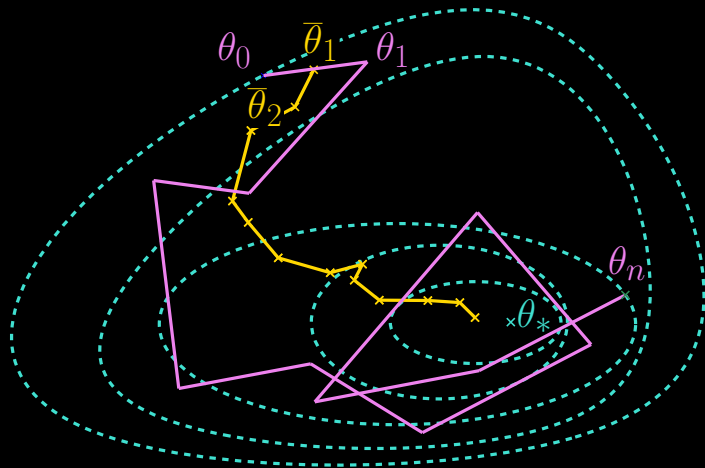
Constant learning rate SGD: convergence in the non-quadratic case



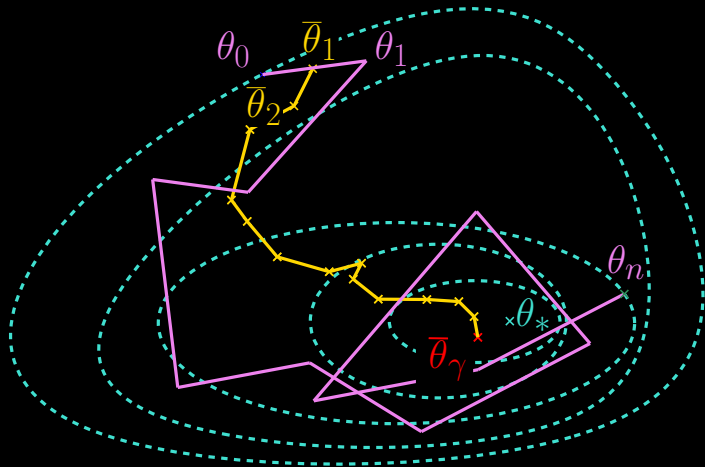
Constant learning rate SGD: convergence in the non-quadratic case



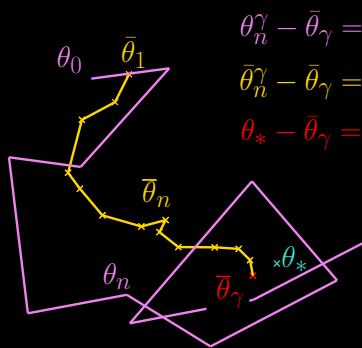
Constant learning rate SGD: convergence in the non-quadratic case



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



Richardson extrapolation



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

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

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

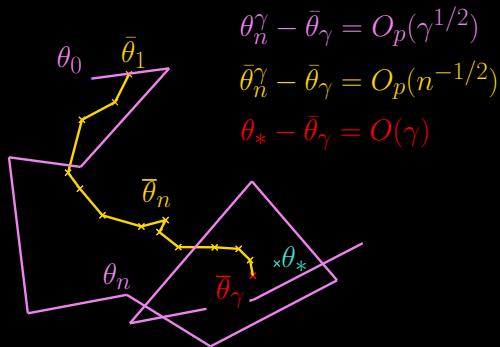
$$\bullet \theta_*$$

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

Recovering convergence closer to θ_* by **Richardson extrapolation**

$$2\bar{\theta}_n^\gamma - \bar{\theta}_n^{2\gamma}$$

Richardson extrapolation



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

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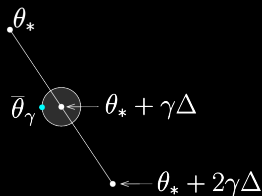
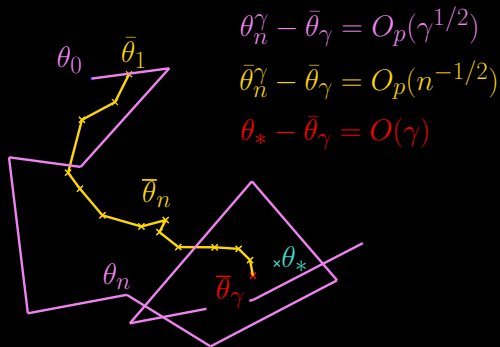
$$\theta_*$$

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

Recovering convergence closer to θ_* by **Richardson extrapolation**

$$2\bar{\theta}_n^\gamma - \bar{\theta}_n^{2\gamma}$$

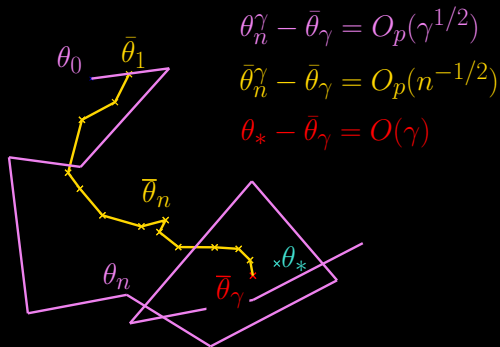
Richardson extrapolation



Recovering convergence closer to θ_* by **Richardson extrapolation**

$$2\bar{\theta}_n^\gamma - \bar{\theta}_n^{2\gamma}$$

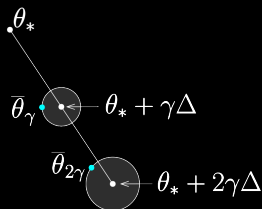
Richardson extrapolation



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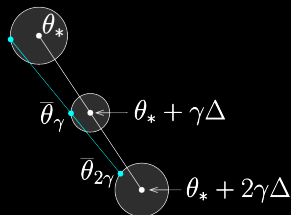
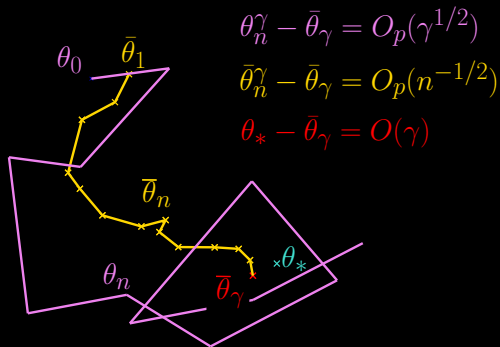
$$\theta_* - \bar{\theta}_\gamma = O(\gamma)$$



Recovering convergence closer to θ_* by **Richardson extrapolation**

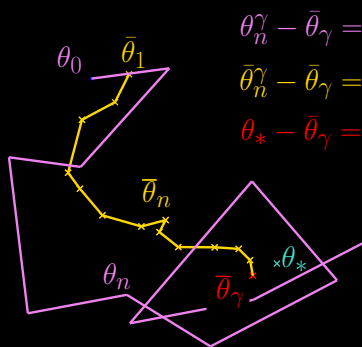
$$2\bar{\theta}_n^\gamma - \bar{\theta}_n^{2\gamma}$$

Richardson extrapolation



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

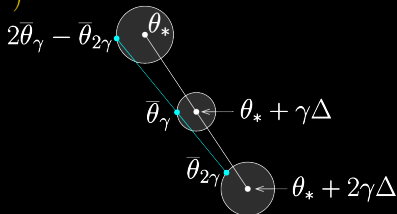
Richardson extrapolation



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

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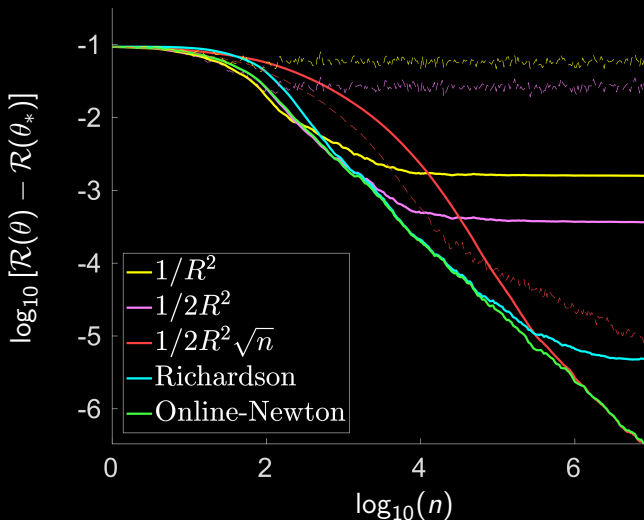
$$\theta_* - \bar{\theta}_\gamma = O(\gamma)$$



Recovering convergence closer to θ_* by **Richardson extrapolation**

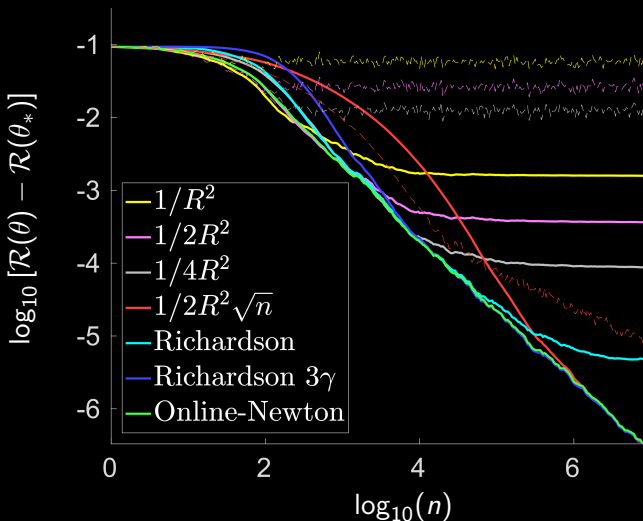
$$2\bar{\theta}_n^\gamma - \bar{\theta}_n^{2\gamma}$$

Experiments: smaller dimension



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

Experiments: Double Richardson



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

“Richardson 3γ ”: 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 γ 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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