Optimization for Machine Learning

Stochastic Gradient Methods

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ENS ÉCOLE NORMALE SUPÉRIEURE

MINES ParisTech

Master IASD: AI Systems and Data Science, 2019

Core Info

- **Where**: ENS: 07/11 amphi Langevin, 03/12 U209, 05/12 amphi Langevin.

- **Online:** Teaching materials for these 3 classes:
  https://gowerrobert.github.io/

- **Google docs with course info:** Can also be found on
  https://gowerrobert.github.io/

Outline of my three classes

- 07/11/19 Foundations and the empirical risk problem, revision probability, SGD (Stochastic Gradient Descent) for ridge regression
- 03/12/19 (**TODAY**) SGD for convex optimization. Theory, variants including averaging, decreasing stepsizes and momentum.
- 05/12/19 Lab on SGD and variants **BRING LAPTOPS!**

Solving the Finite Sum Training Problem

Recap

Training Problem

$$\underbrace{\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} \ell\left(h_w(x^i), y^i\right)}_{L(w) = loss} + \lambda R(w) =: f(w)$$

General methods

$\min f(w)$

- Gradient Descent

Two parts

$\min L(w) + \lambda R(w)$

- Proximal gradient (ISTA)
- Fast proximal gradient (FISTA)

Optimization Sum of Terms

A Datum Function

$$f_i(w) := \ell\left(h_w(x^i), y^i\right) + \lambda R(w)$$

$$\begin{aligned}\frac{1}{n}\sum_{i=1}^{n} \ell\left(h_w(x^i), y^i\right) + \lambda R(w) &= \frac{1}{n}\sum_{i=1}^{n} \left(\ell\left(h_w(x^i), y^i\right) + \lambda R(w)\right) \\ &= \frac{1}{n}\sum_{i=1}^{n} f_i(w)\end{aligned}$$

Finite Sum Training Problem

$$\min_{w \in \mathbf{R}^d} \frac{1}{n}\sum_{i=1}^{n} f_i(w) =: f(w)$$

Can we use this sum structure?

The Training Problem

Solving the *training problem*: $$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} f_i(w)$$

Reference method: Gradient descent

$$\nabla \left(\frac{1}{n} \sum_{i=1}^{n} f_i(w) \right) = \frac{1}{n} \sum_{i=1}^{n} \nabla f_i(w)$$

Gradient Descent Algorithm

Set $w^0 = 0$, choose $\alpha > 0$.

for $t = 0, 1, 2, \ldots, T-1$

$$w^{t+1} = w^t - \frac{\alpha}{n} \sum_{i=1}^{n} \nabla f_i(w^t)$$

Output w^T

The Training Problem

Solving the *training problem*:

$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} f_i(w)$$

Problem with Gradient Descent:
Each iteration requires computing a gradient $\nabla f_i(w)$ for each data point. One gradient for each cat on the internet!

Gradient Descent Algorithm

Set $w^0 = 0$, choose $\alpha > 0$.
for $t = 0, 1, 2, \ldots, T$
$$w^{t+1} = w^t - \frac{\alpha}{n} \sum_{i=1}^{n} \nabla f_i(w^t)$$
Output w^T

Stochastic Gradient Descent

Is it possible to design a method that uses only the gradient of a **single** data function $f_i(w)$ at each iteration?

Stochastic Gradient Descent

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Unbiased Estimate

Let j be a random index sampled from $\{1, \dots, n\}$ selected uniformly at random. Then

$$\mathbb{E}_j[\nabla f_j(w)] = \frac{1}{n}\sum_{i=1}^{n} \nabla f_i(w) = \nabla f(w)$$

Stochastic Gradient Descent

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Use $\nabla f_j(w) \approx \nabla f(w)$

Stochastic Gradient Descent

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Use $\nabla f_j(w) \approx \nabla f(w)$

EXE: Let $\sum_{i=1}^{n} p_i = 1$ and $j \sim p_j$. Show $\mathbb{E}[\nabla f_j(w)/(np_j)] = \nabla f(w)$

Stochastic Gradient Descent

SGD 0.0 Constant stepsize

Set $w^0 = 0$, choose $\alpha > 0$

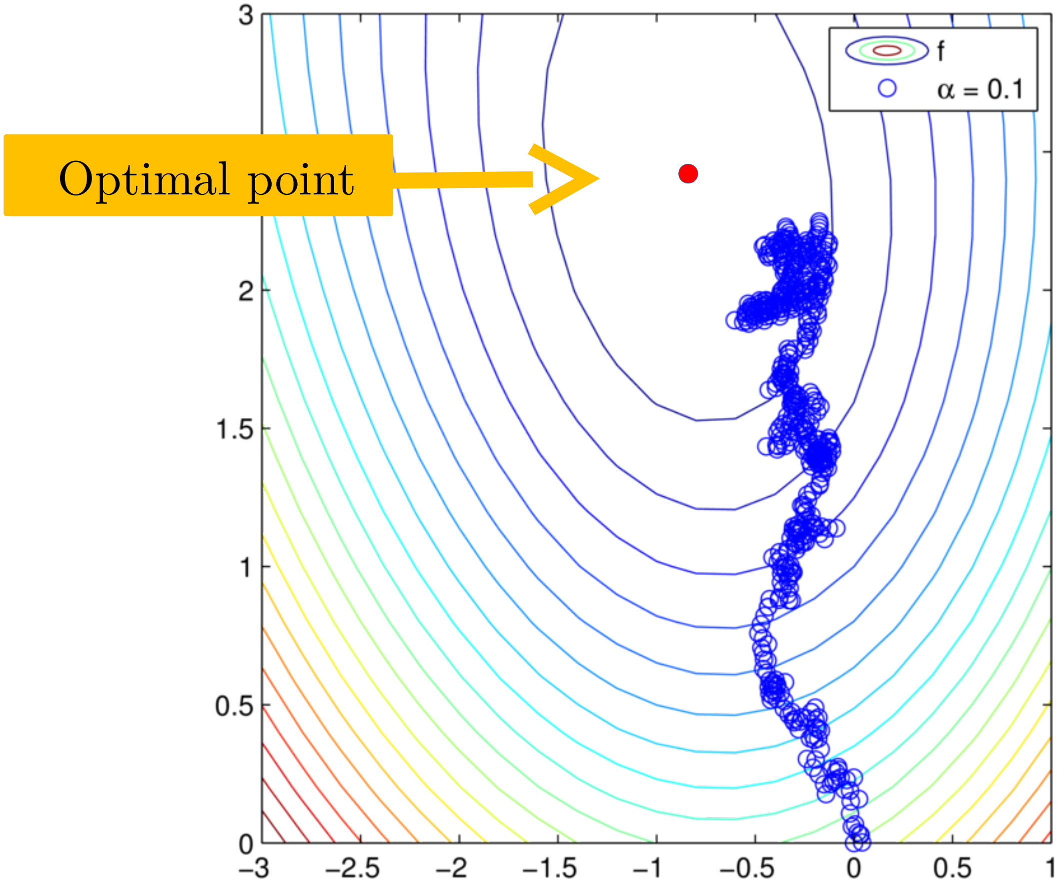
for $t = 0, 1, 2, \ldots, T-1$

  sample $j \in \{1, \ldots, n\}$

  $w^{t+1} = w^t - \alpha \nabla f_j(w^t)$

Output w^T

Stochastic Gradient Descent



Assumptions for Convergence

Strong Convexity

$$f(y) \geq f(w) + \langle \nabla f(w), y - w \rangle + \frac{\lambda}{2}||y - w||_2^2, \quad \forall w, y$$

$$y = w^*$$

$$2\langle \nabla f(w), w - w^* \rangle \geq \lambda ||w - w^*||_2^2$$

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Expected Bounded Stochastic Gradients

$$\mathbb{E}_j[||\nabla f_j(w^t)||_2^2] \leq B^2, \text{ for all iterates } w^t \text{ of SGD}$$

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Complexity / Convergence

Theorem

If $0 < \alpha \leq \frac{1}{\lambda}$ then the iterates of the SGD 0.0 method satisfy

$$\mathbb{E}\left[||w^t - w^*||_2^2\right] \leq (1-\alpha\lambda)^t ||w^0 - w^*||_2^2 + \frac{\alpha}{\lambda} B^2$$

EXE: Do exercises on convergence of random sequences.

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Shows that $\alpha \approx \frac{1}{\lambda}$

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Shows that $\alpha \approx \frac{1}{\lambda}$

Shows that $\alpha \approx 0$

EXE: Do exercises on convergence of random sequences.

Proof:

$$
\begin{aligned}
||w^{t+1} - w^*||_2^2 &= ||w^t - w^* - \alpha \nabla f_j(w^t)||_2^2 \\
&= ||w^t - w^*||_2^2 - 2\alpha \langle \nabla f_j(w^t), w^t - w^* \rangle + \alpha^2 ||\nabla f_j(w^t)||_2^2.
\end{aligned}
$$

Taking expectation with respect to j

Unbiased estimator

$$
\begin{aligned}
\mathbb{E}_j \left[||w^{t+1} - w^*||_2^2 \right] &= ||w^t - w^*||_2^2 - 2\alpha \langle \nabla f(w^t), w^t - w^* \rangle + \alpha^2 \mathbb{E}_j \left[||\nabla f_j(w^t)||_2^2 \right] \\
&\leq ||w^t - w^*||_2^2 - 2\alpha \langle \nabla f(w^t), w^t - w^* \rangle + \alpha^2 B^2 \\
&\leq (1 - \alpha\lambda) ||w^t - w^*||_2^2 + \alpha^2 B^2
\end{aligned}
$$

Strong conv.

Bounded
Stoch grad

Taking total expectation

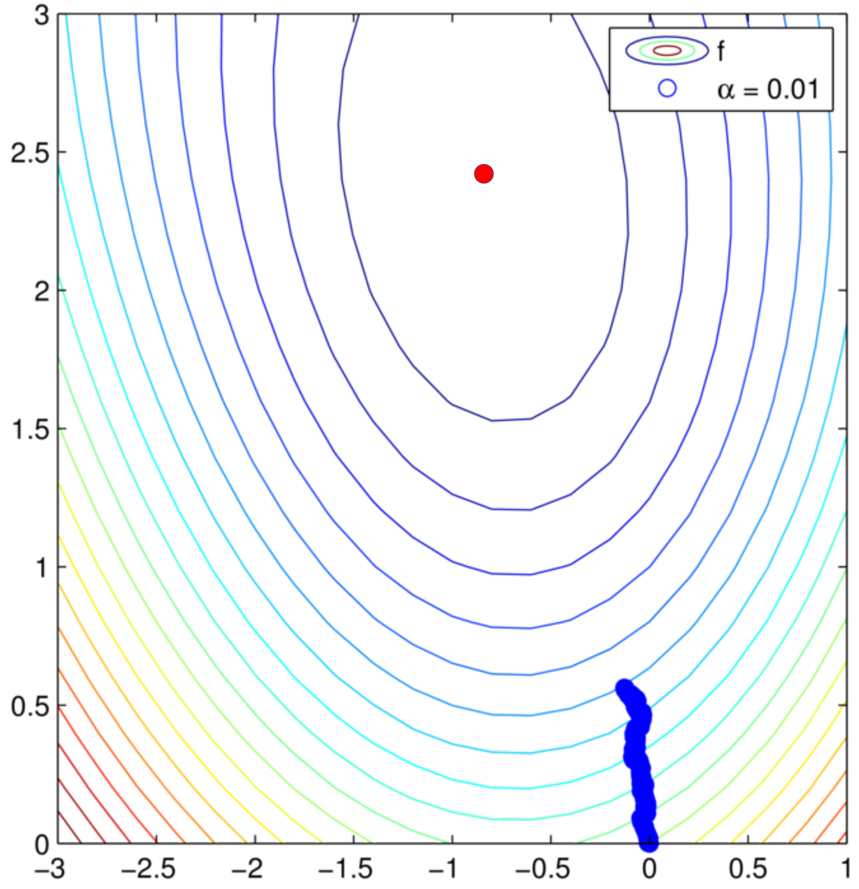
$$
\begin{aligned}
\mathbb{E} \left[||w^{t+1} - w^*||_2^2 \right] &\leq (1 - \alpha\lambda) \mathbb{E} \left[||w^t - w^*||_2^2 \right] + \alpha^2 B^2 \\
&= (1 - \alpha\lambda)^{t+1} ||w^0 - w^*||_2^2 + \textstyle\sum_{i=0}^t (1 - \alpha\lambda)^i \alpha^2 B^2
\end{aligned}
$$

Using the geometric series sum $\displaystyle\sum_{i=0}^{t} (1 - \alpha\lambda)^i = \frac{1 - (1 - \alpha\lambda)^{t+1}}{\alpha\lambda} \leq \frac{1}{\alpha\lambda}$

$$
\mathbb{E} \left[||w^{t+1} - w^*||_2^2 \right] \leq (1 - \alpha\lambda)^{t+1} ||w^0 - w^*||_2^2 + \tfrac{\alpha}{\lambda} B^2
$$

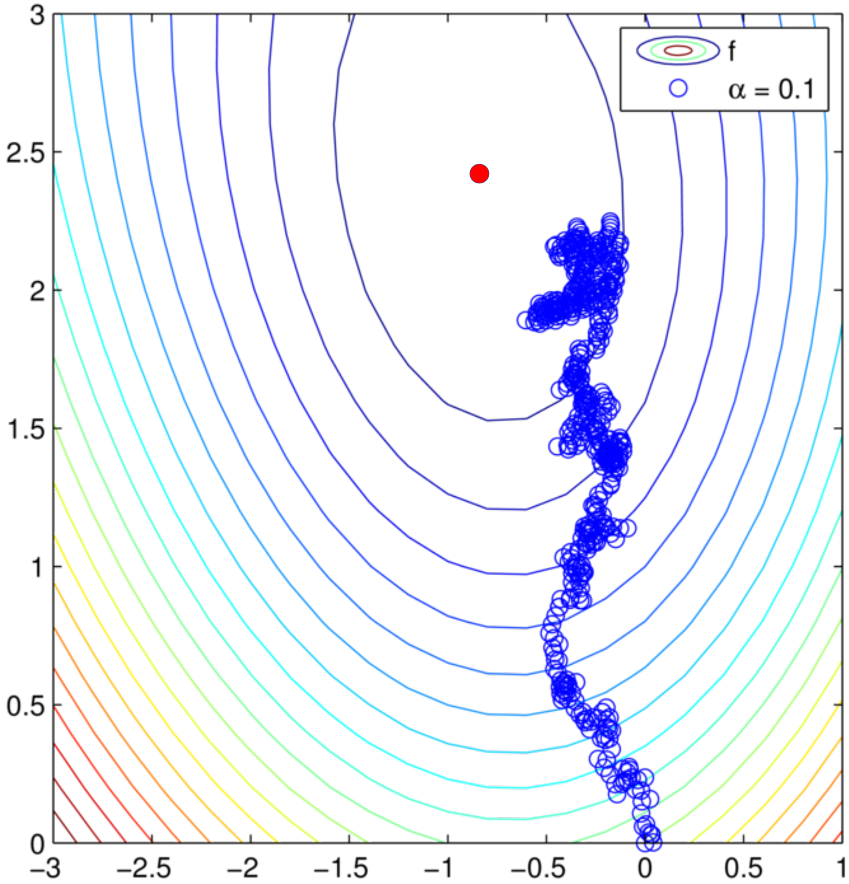
Stochastic Gradient Descent

α =0.01



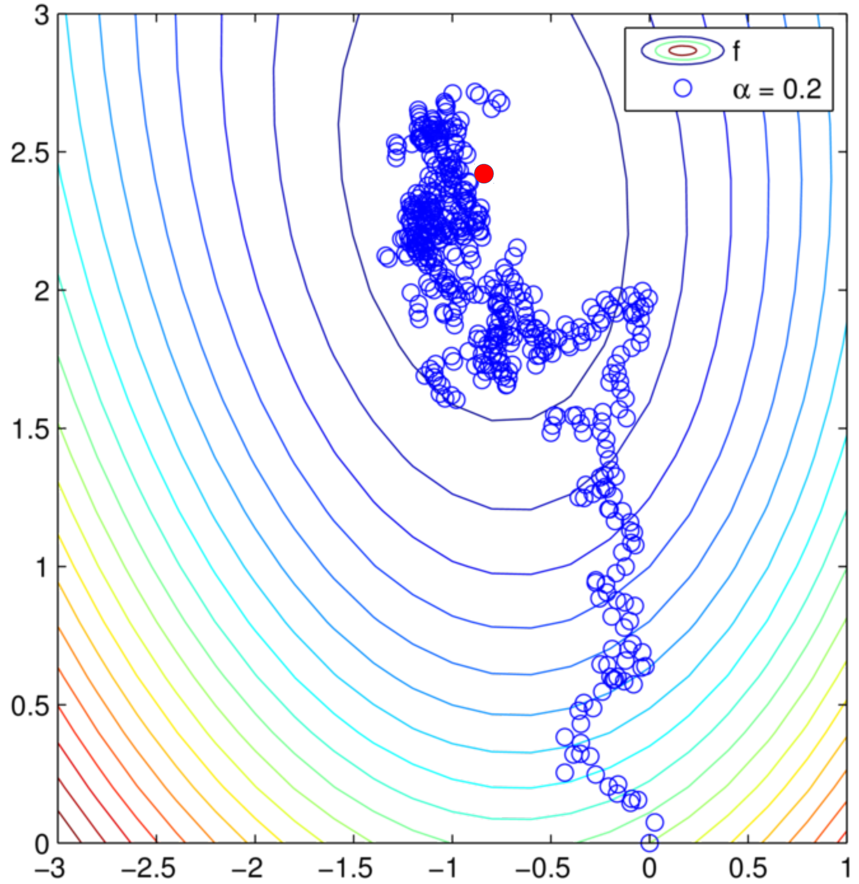
Stochastic Gradient Descent

α =0.1



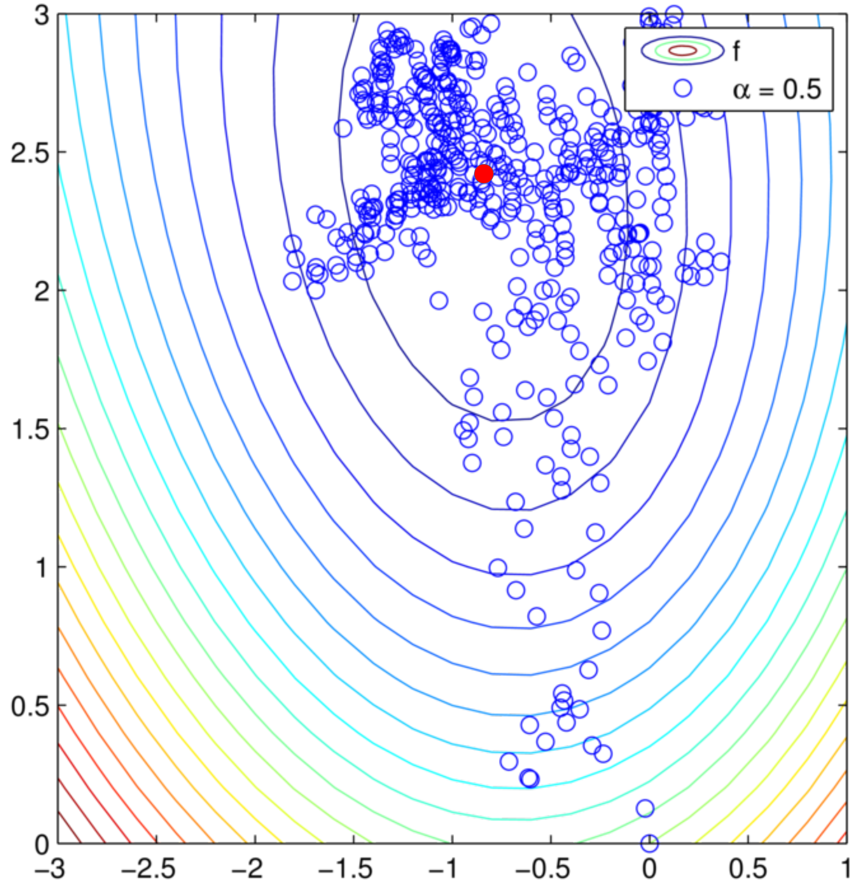
Stochastic Gradient Descent

α =0.2



Stochastic Gradient Descent

α =0.5



Assumptions for Convergence

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$$\Big\Downarrow \; y = w^*$$

$$2\langle \nabla f(w), w - w^* \rangle \geq \lambda ||w - w^*||_2^2$$

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$$\mathbb{E}_j[||\nabla f_j(w^t)||_2^2] \leq B^2, \text{ for all iterates } w^t \text{ of SGD}$$

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~~**Expected Bounded Stochastic Gradients**~~

~~$\mathbb{E}_j[||\nabla f_j(w^t)||_2^2] \leq B^2$, for all iterates w^t of SGD~~

EXE:
Let $A \in \mathbb{R}^{n \times d}$, $f_j(w) = (A_{j:}w - b_j)^2$. $\quad \max_w \mathbb{E}_{j \sim \frac{1}{n}}[\|\nabla f_j(w)\|^2] \; = ?$

EXE:
Let $A \in \mathbb{R}^{n\times d}$, $f_j(w) = (A_{j:}w - b_j)^2$. $\max_w \mathbb{E}_{j\sim\frac{1}{n}}[\|\nabla f_j(w)\|^2] = ?$

Proof: $\max_w \mathbb{E}_{j\sim\frac{1}{n}}[\|\nabla f_j(w)\|^2] = \infty$, indeed since

$$
\begin{aligned}
\|\nabla f_j(w)\|^2 &= 4\|A_{j:}^\top(A_{j:}w - b_j)\|^2 \\
&= 4\|A_{j:}\|^2(A_{j:}w - b_j)^2 \\
&= 4(\hat{A}_{j:}w - \hat{b}_j)^2 \qquad \text{where } \hat{A}_{j:} := A_{j:}\|A_{j:}\|, \quad \hat{b}_j := b_j\|A_{j:}\|
\end{aligned}
$$

Taking expectation

$$\mathbb{E}_{j\sim\frac{1}{n}}\|\nabla f_j(w)\|^2 = \frac{1}{n}\sum_{j=1}^n 4(\hat{A}_{j:}w - \hat{b}_j)^2 = \frac{1}{n}\|\hat{A}w - \hat{b}\|^2$$

$$\lim_{w\to\infty}\|\hat{A}w - b\|^2 = \infty$$

Realistic assumptions for Convergence

Strongly quasi-convexity

$$f(w^*) \geq f(w) + \langle \nabla f(w), w^* - w \rangle + \frac{\mu}{2} ||w^* - w||_2^2, \quad \forall w$$

Each f_i is convex and L_i smooth

$$f_i(y) \leq f_i(w) + \langle \nabla f_i(w), y - w \rangle + \frac{L_i}{2} ||y - w||_2^2, \quad \forall w$$

$$L_{\max} := \max_{i=1,\ldots,n} L_i$$

Definition: Gradient Noise

$$\sigma^2 \quad := \quad \mathbb{E}_j [||\nabla f_j(w^*)||_2^2]$$

1. $f(w) = \frac{1}{2n}||Aw - y||_2^2 + \frac{\lambda}{2}||w||_2^2 = \frac{1}{n}\sum_{i=1}^{n}(\frac{1}{2}(A_{i:}^\top w - y_i)^2 + \frac{\lambda}{2}||w||_2^2)$

Assumptions for Convergence

EXE: Calculate the L_i's and $L_{\max}$ for

$$1. \quad f(w) = \frac{1}{2n}||Aw - y||_2^2 + \frac{\lambda}{2}||w||_2^2$$

HINT: A twice differentiable f_i is L_i - smooth if and only if

$$\nabla^2 f_i(w) \preceq L_i\, I \quad \Leftrightarrow \quad v^\top \nabla^2 f_i(w) v \leq L_i \|v\|^2, \forall v$$

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$$= \frac{1}{n}\sum_{i=1}^{n} f_i(w)$$

$$\nabla^2 f_i(w) = A_{i:}A_{i:}^\top + \lambda \quad \preceq \quad (||A_{i:}||_2^2 + \lambda)I \quad = \quad L_i\, I$$

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$$L_{\max} \quad = \quad \max_{i=1,\ldots,n}(||A_{i:}||_2^2 + \lambda) \quad = \max_{i=1,\ldots,n} ||A_{i:}||_2^2 + \lambda$$

Assumptions for Convergence

EXE: Calculate the L_i's and $L_{\max}$ for

2. $$f(w) = \frac{1}{n}\sum_{i=1}^{n} \ln(1 + e^{-y_i\langle w, a_i\rangle}) + \frac{\lambda}{2}||w||_2^2$$

Assumptions for Convergence

EXE: Calculate the L_i's and $L_{\max}$ for

$$2. \quad f(w) = \frac{1}{n}\sum_{i=1}^{n} \ln(1+e^{-y_i\langle w, a_i\rangle}) + \frac{\lambda}{2}||w||_2^2$$

$$2. \quad f_i(w) = \ln(1+e^{-y_i\langle w, a_i\rangle}) + \frac{\lambda}{2}||w||_2^2,$$

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$$2. \quad f_i(w) = \ln(1+e^{-y_i\langle w,a_i\rangle}) + \frac{\lambda}{2}||w||_2^2,$$

$$\nabla f_i(w) = \frac{-y_i a_i e^{-y_i\langle w,a_i\rangle}}{1+e^{-y_i\langle w,a_i\rangle}} + \lambda w$$

$$\nabla^2 f_i(w) = a_i a_i^\top \left(\frac{(1+e^{-y_i\langle w,a_i\rangle})e^{-y_i\langle w,a_i\rangle}}{(1+e^{-y_i\langle w,a_i\rangle})^2} - \frac{e^{-2y_i\langle w,a_i\rangle}}{(1+e^{-y_i\langle w,a_i\rangle})^2} \right) + \lambda I$$

$$= a_i a_i^\top \frac{e^{-y_i\langle w,a_i\rangle}}{(1+e^{-y_i\langle w,a_i\rangle})^2} + \lambda I \quad \preceq \quad \left(\frac{||a_i||_2^2}{4} + \lambda \right) I = L_i \, I$$

Relationship between smoothness constants

EXE: Let f be differentiable and convex. Show that $f(w)$ is L–smooth with

$$L = \max_{w \in \mathbb{R}^d} \lambda_{\max}(\nabla^2 f(w))$$

Thus $f_i(w)$ is L_i–smooth with $L_i = \max_{w \in \mathbb{R}^d} \lambda_{\max}(\nabla^2 f_i(w))$ show that

$$L \quad \leq \quad \frac{1}{n}\sum_{i=1}^n L_i \quad \leq \quad L_{\max} := \max_{i=1,\ldots,n} L_i$$

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$$L \quad \leq \quad \frac{1}{n}\sum_{i=1}^n L_i \quad \leq \quad L_{\max} := \max_{i=1,\ldots,n} L_i$$

Proof: From the Hessian definition of smoothness

$$\nabla^2 f(w) \quad \preceq \quad \lambda_{\max}(\nabla^2 f(w)) I \quad \preceq \quad \max_{w \in \mathbb{R}^d} \lambda_{\max}(\nabla^2 f(w)) I$$

Furthermore

$$\lambda_{\max}(\nabla^2 f(w)) = \lambda_{\max}\left(\frac{1}{n}\sum_{i=1}^n \nabla^2 f_i(w)\right) \leq \frac{1}{n}\sum_{i=1}^n \lambda_{\max}(\nabla^2 f_i(w)) \leq \frac{1}{n}\sum_{i=1}^n L_i$$

Which follows since the largest eigenvalue function is convex over psd matrices. Now take the max over w, *then* max over i.

Complexity / Convergence

Theorem.

Let f be μ–strongly quasi-convex and f_i be L_i–smooth.

If $0 < \alpha \leq \frac{1}{2L_{\max}}$ then the iterates of the SGD 0.0 satisfy

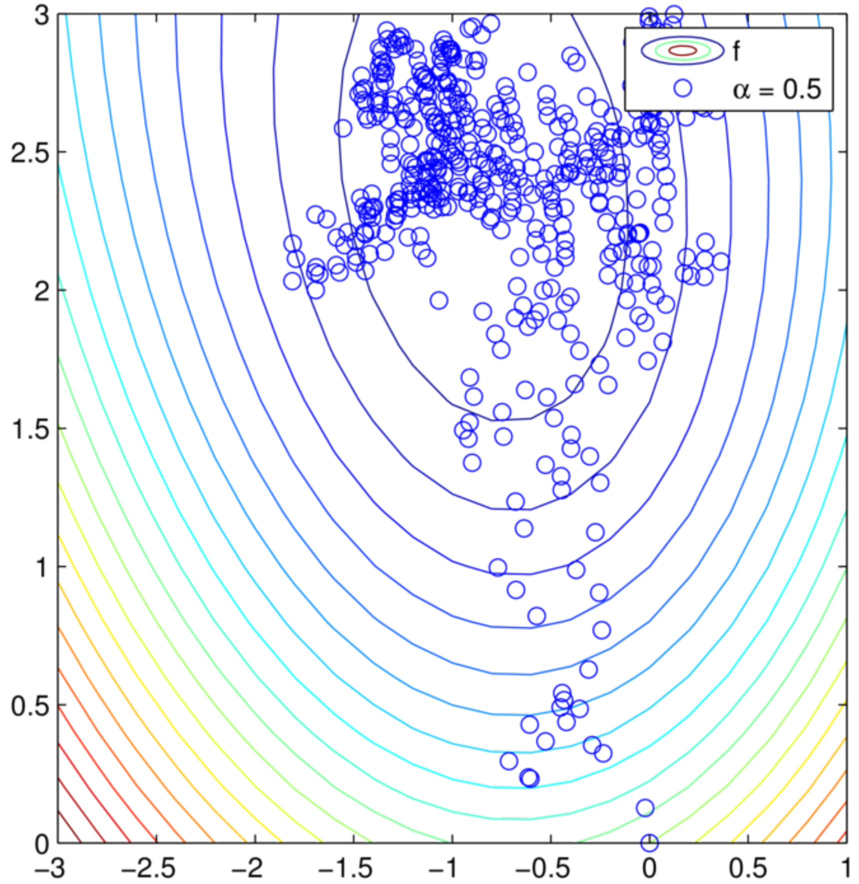
$$\mathbb{E}\left[||w^t - w^*||_2^2\right] \leq (1-\alpha\mu)^t ||w^0 - w^*||_2^2 + \frac{2\alpha}{\mu}\sigma^2$$

EXE: The steps of the proof are given in the SGD_proof exercise list for homework!

RMG, N. Loizou, X. Qian, A. Sailanbayev, E. Shulgin, P. Richtarik (2019) ICML 2019
SGD: General Analysis and Improved Rates.

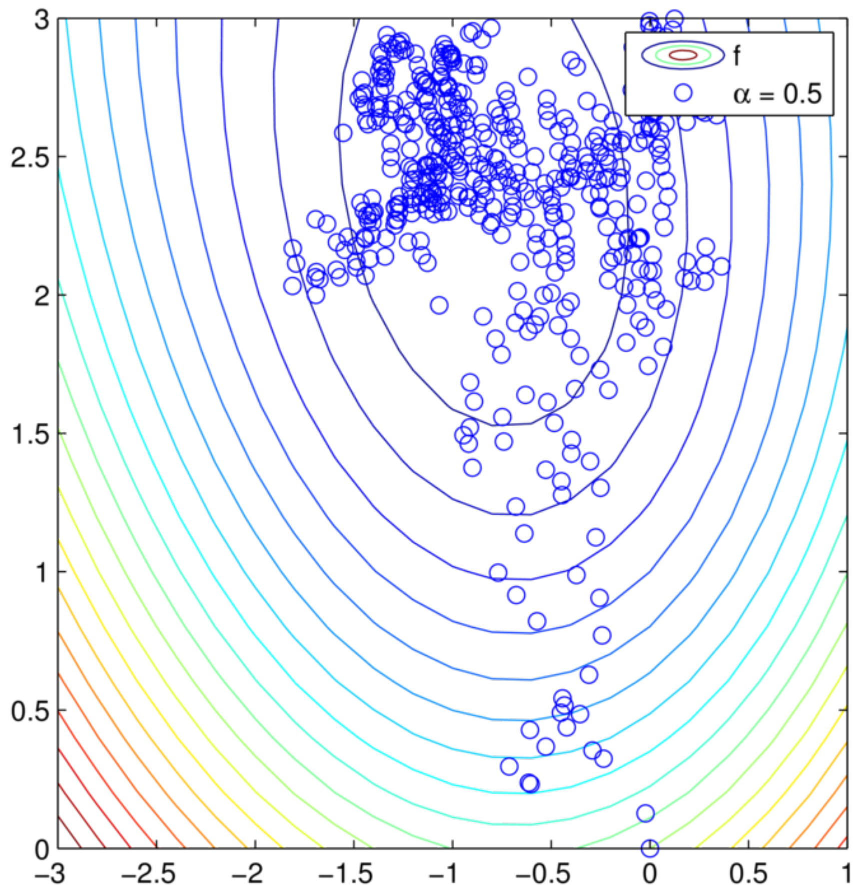
Stochastic Gradient Descent

α =0.5



Stochastic Gradient Descent

α =0.5



1) Start with big steps and end with smaller steps

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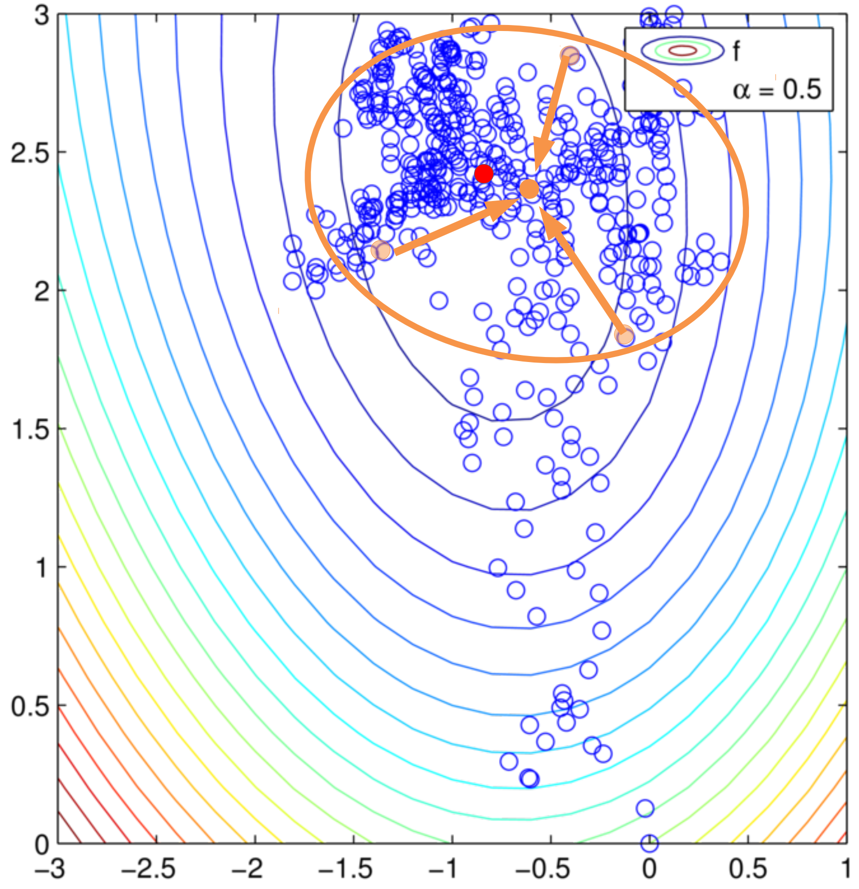

1) Start with big steps and end with smaller steps

2) Try averaging the points

SGD shrinking stepsize

SGD 1.0: Descreasing stepsize

Set $w^0 = 0$

Choose $\alpha_t > 0,\ \alpha_t \rightarrow 0,\ \sum_{t=0}^{\infty} \alpha_t = \infty$

for $t = 0, 1, 2, \ldots, T-1$

  sample $j \in \{1, \ldots, n\}$

  $w^{t+1} = w^t - \alpha_t \nabla f_j(w^t)$

Output w^T

Shrinking Stepsize

SGD shrinking stepsize

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Shrinking Stepsize

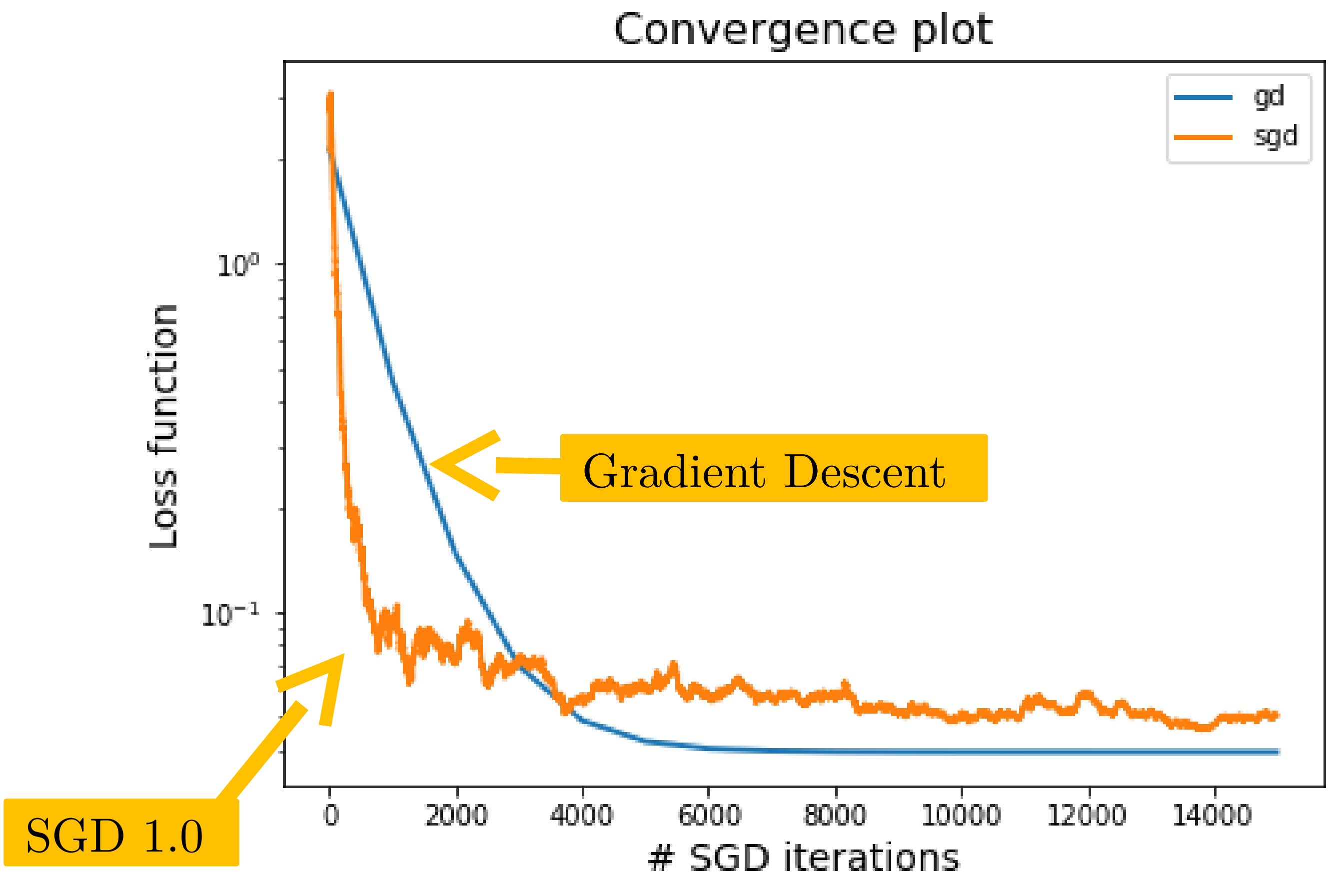
How should we sample j ?

How fast $\alpha_t \to 0$?

Does this converge?

SGD with shrinking stepsize

Compared with Gradient Descent



SGD with shrinking stepsize
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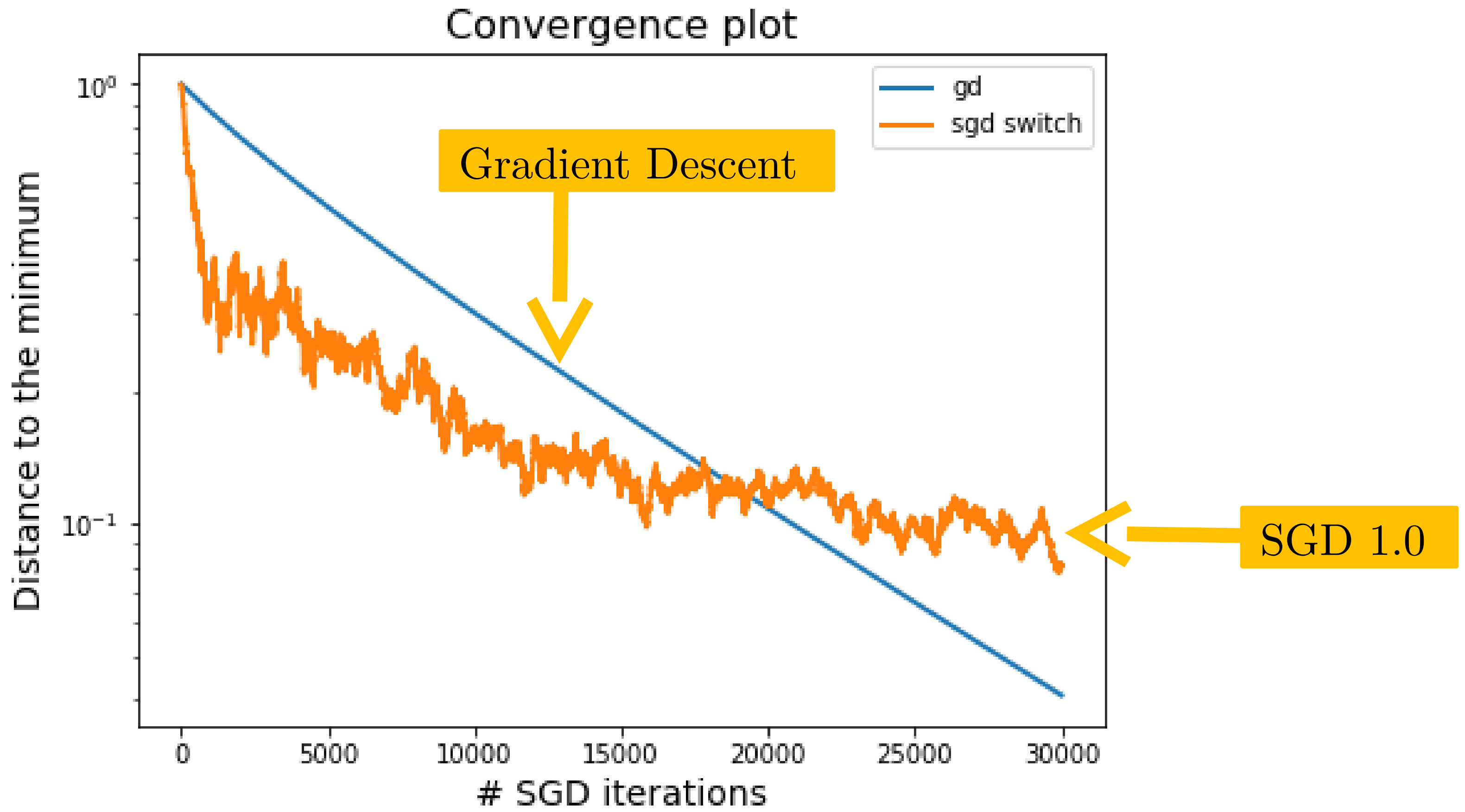

Complexity / Convergence

$$L_{\max} := \max_{i=1,\ldots,n} L_i$$

Theorem for shrinking stepsizes

Let f be μ–strongly quasi-convex and f_i be L_i–smooth.

Let $\mathcal{K} := L_{\max}/\mu$ and let

$$\alpha^t = \begin{cases} \frac{1}{2L_{\max}} & \text{for} \quad t \leq 4\lceil \mathcal{K} \rceil \\ \frac{2t+1}{(t+1)^2\mu} & \text{for} \quad t > 4\lceil \mathcal{K} \rceil. \end{cases}$$

If $t \geq 4\lceil \mathcal{K} \rceil$, then SGD 1.0 satifies

$$\mathbb{E}\|w^t - w^*\|^2 \leq \frac{\sigma^2}{\mu^2}\frac{8}{t} + \frac{16}{e^2}\frac{\lceil \mathcal{K} \rceil^2}{t^2}\|w^0 - w^*\|^2$$

$$O\left(\frac{1}{t}\right)$$

Iteration complexity $O\left(\frac{1}{\epsilon}\right)$

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If $t \geq 4\lceil \mathcal{K} \rceil$, then SGD 1.0 satifies

$\alpha^t = O(1/(t+1))$

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$O\left(\frac{1}{t}\right)$ $\Rightarrow$ Iteration complexity $O\left(\frac{1}{\epsilon}\right)$

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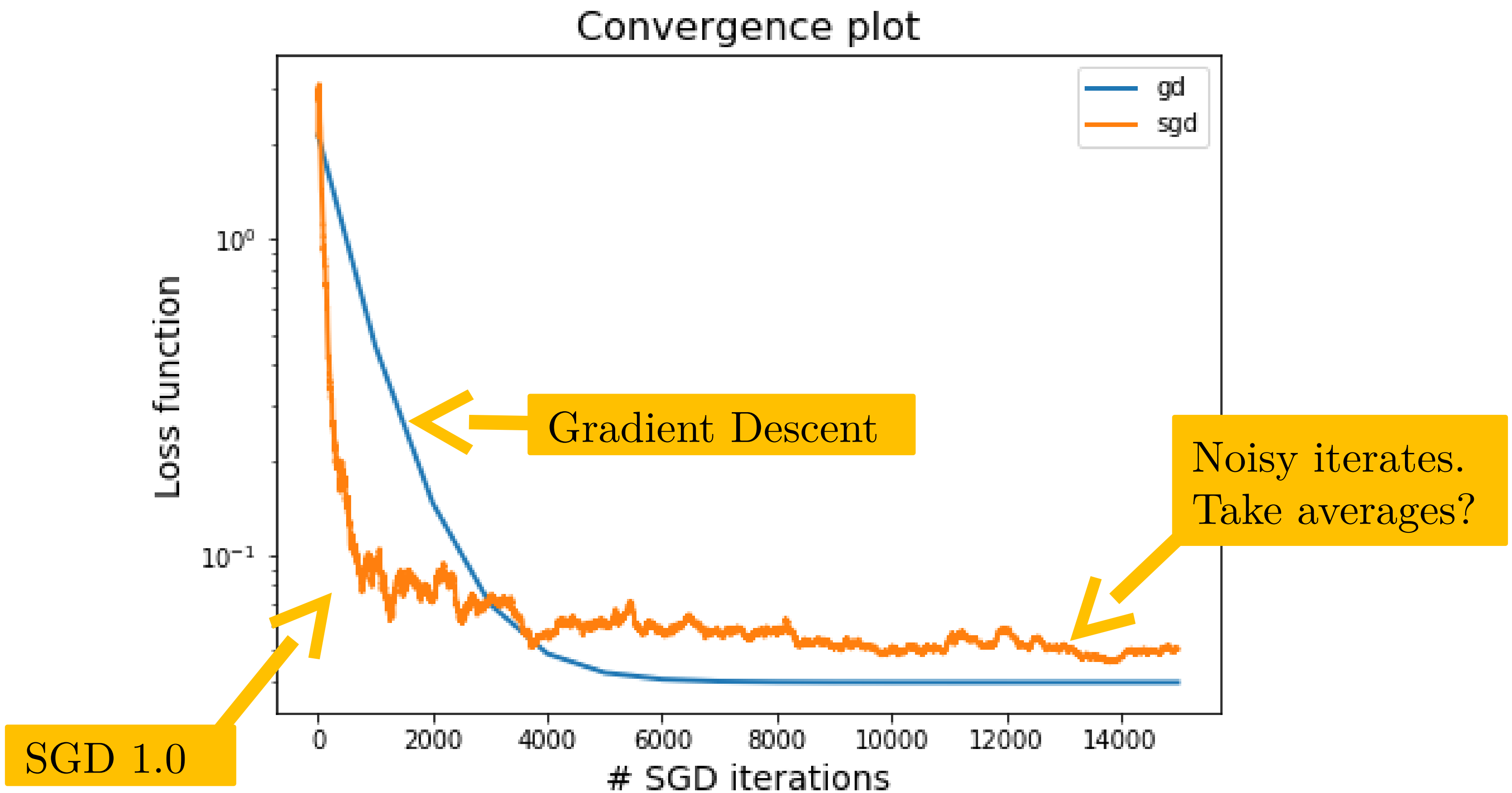
$O\left(\frac{1}{t}\right)$ $\Rightarrow$ Iteration complexity $O\left(\frac{1}{\epsilon}\right)$

In practice $\alpha^t = C/(t+1)$ or $\alpha^t = C/\sqrt{t+1}$ where C is tuned

Stochastic Gradient Descent
Compared with Gradient Descent



SGD with (late start) averaging

SGDA 1.1

Set $w^0 = 0$

Choose $\alpha_t > 0,\ \alpha_t \to 0,\ \sum_{t=0}^{\infty} \alpha_t = \infty$

Choose averaging start $s_0 \in \mathbb{N}$

for $t = 0, 1, 2, \ldots, T-1$

  sample $j \in \{1, \ldots, n\}$

  $w^{t+1} = w^t - \alpha_t \nabla f_j(w^t)$

  if $t > s_0$

    $\overline{w} = \frac{1}{t-s_0} \sum_{i=s_0}^{t} w^t$

  else: $\overline{w} = w$

Output $\overline{w}$

B. T. Polyak and A. B. Juditsky, SIAM Journal on Control and Optimization (1992)
Acceleration of stochastic approximation by averaging

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This is not efficient. How to make this efficient?

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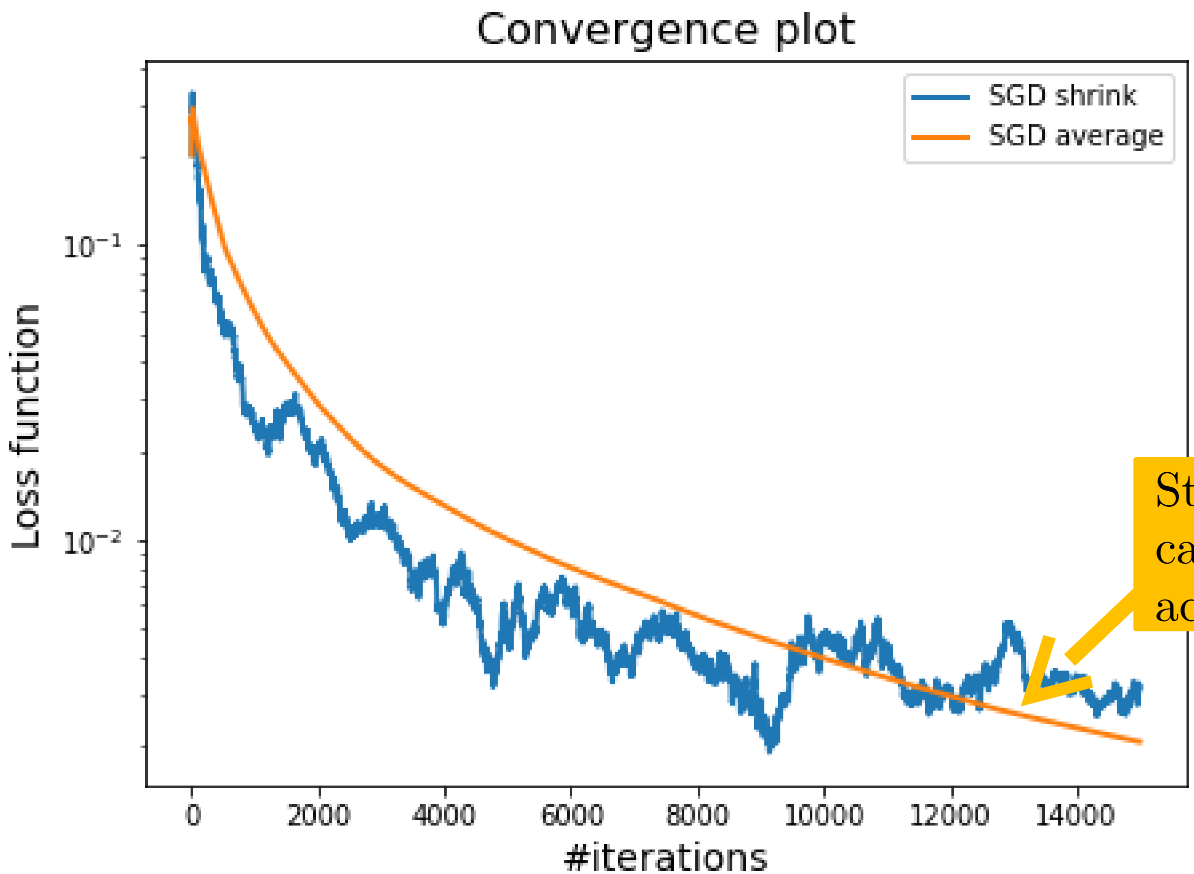
Stochastic Gradient Descent

With and without averaging



Starts slow, but can reach higher accuracy

Stochastic Gradient Descent

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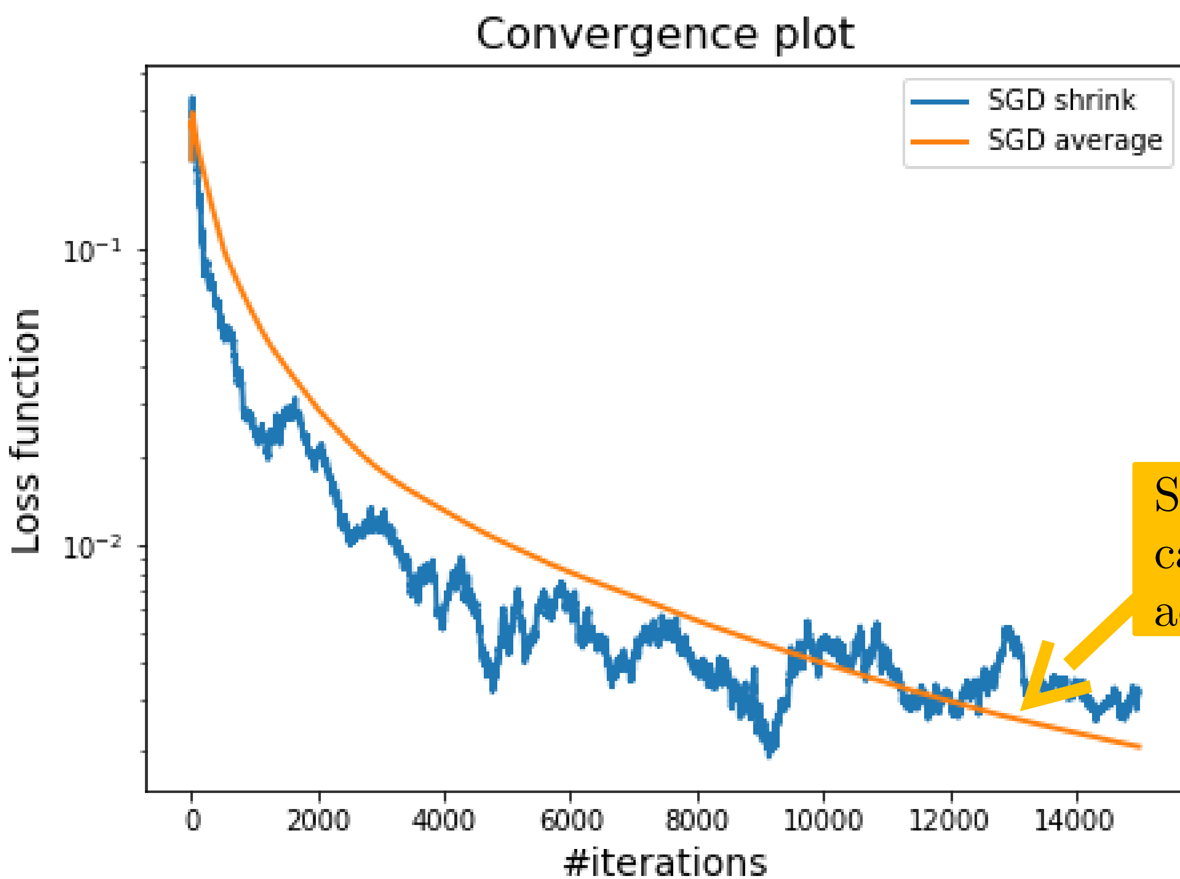
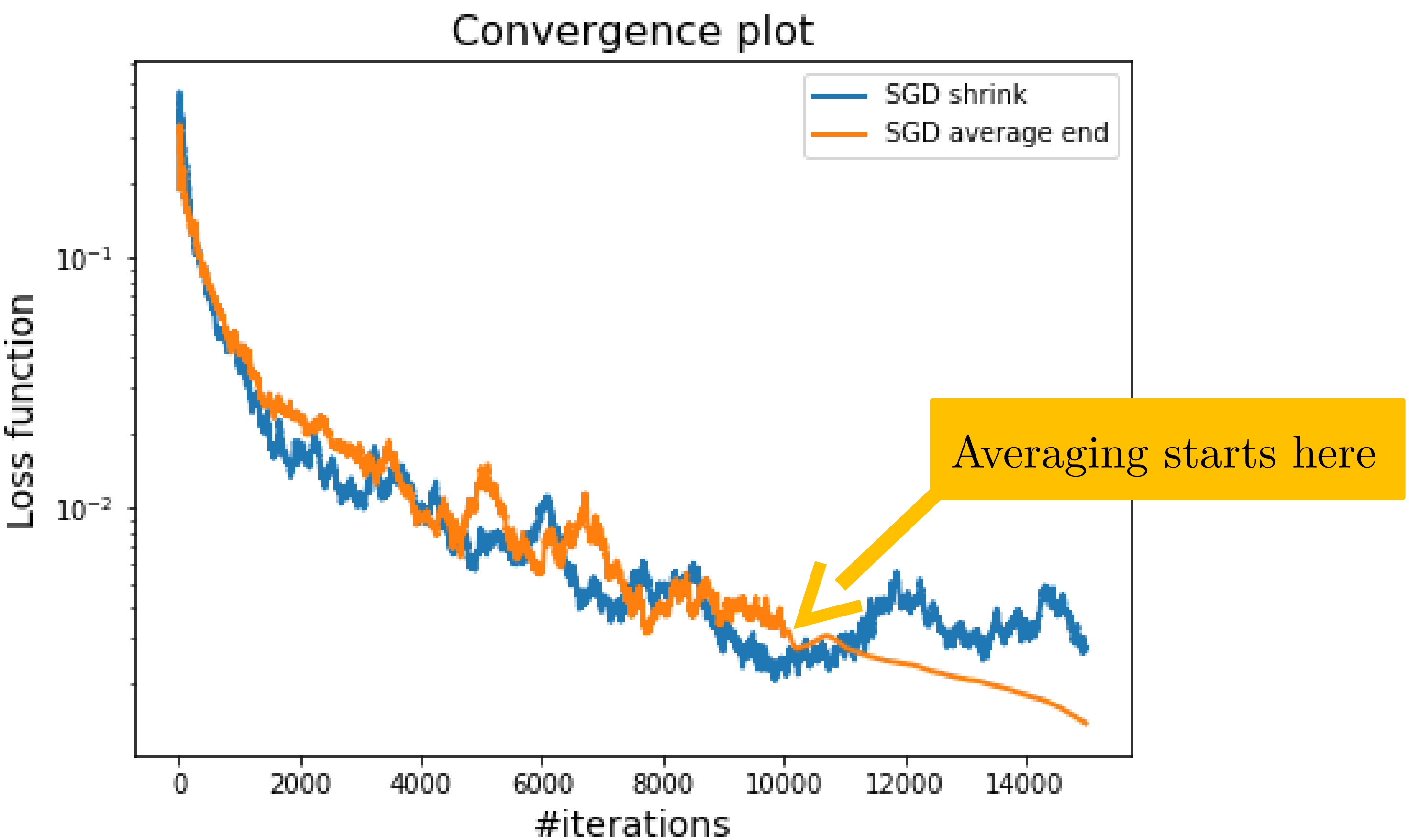


Starts slow, but can reach higher accuracy

Only use averaging towards the end?

Stochastic Gradient Descent

Averaging the last few iterates



Comparison GD and SGD for strongly convex

	SGD	**GD**
Iteration complexity	$O\left(\frac{1}{\epsilon}\right)$	$O\left(\log\left(\frac{1}{\epsilon}\right)\right)$

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*Total complexity = (Iteration complexity) × (Cost of an iteration)

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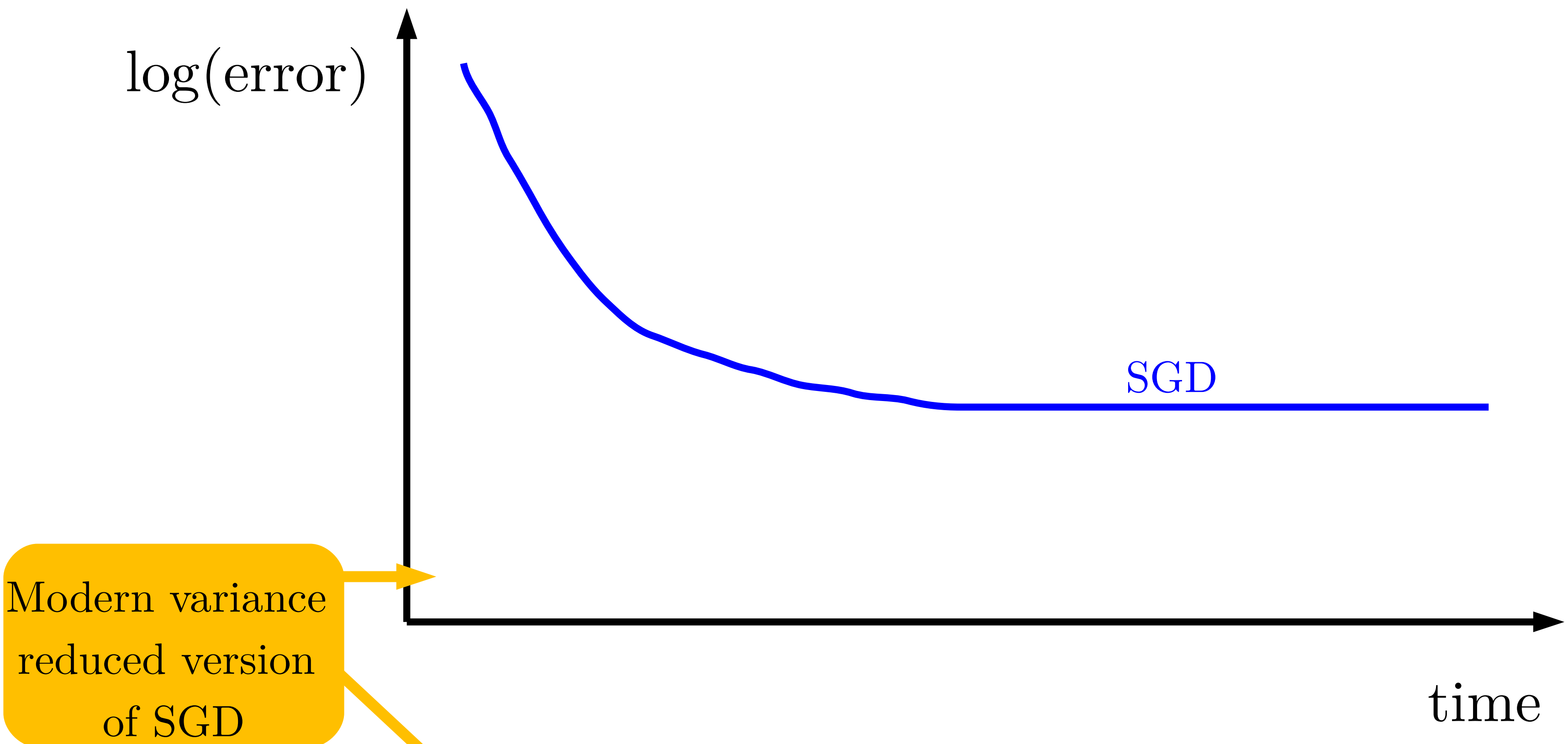
Total complexity*	$O\left(\frac{1}{\epsilon}\right)$	$O\left(n\log\left(\frac{1}{\epsilon}\right)\right)$

What happens if ϵ is small?

What happens if n is big?

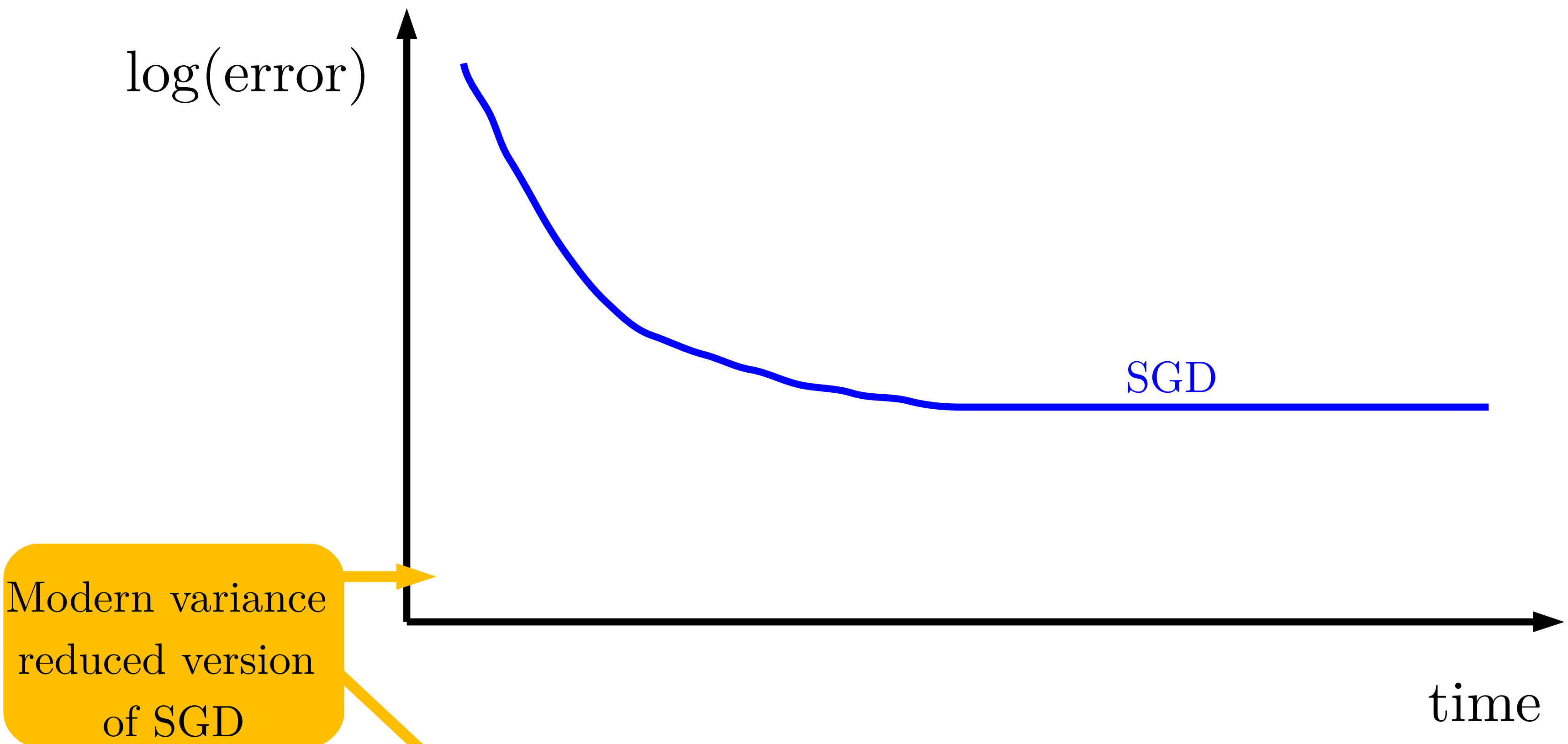
*Total complexity $=$ (Iteration complexity) $\times$ (Cost of an iteration)

Comparison SGD vs GD



M. Schmidt, N. Le Roux, F. Bach (2016)
Mathematical Programming
Minimizing Finite Sums with the Stochastic Average Gradient.

Comparison SGD vs GD



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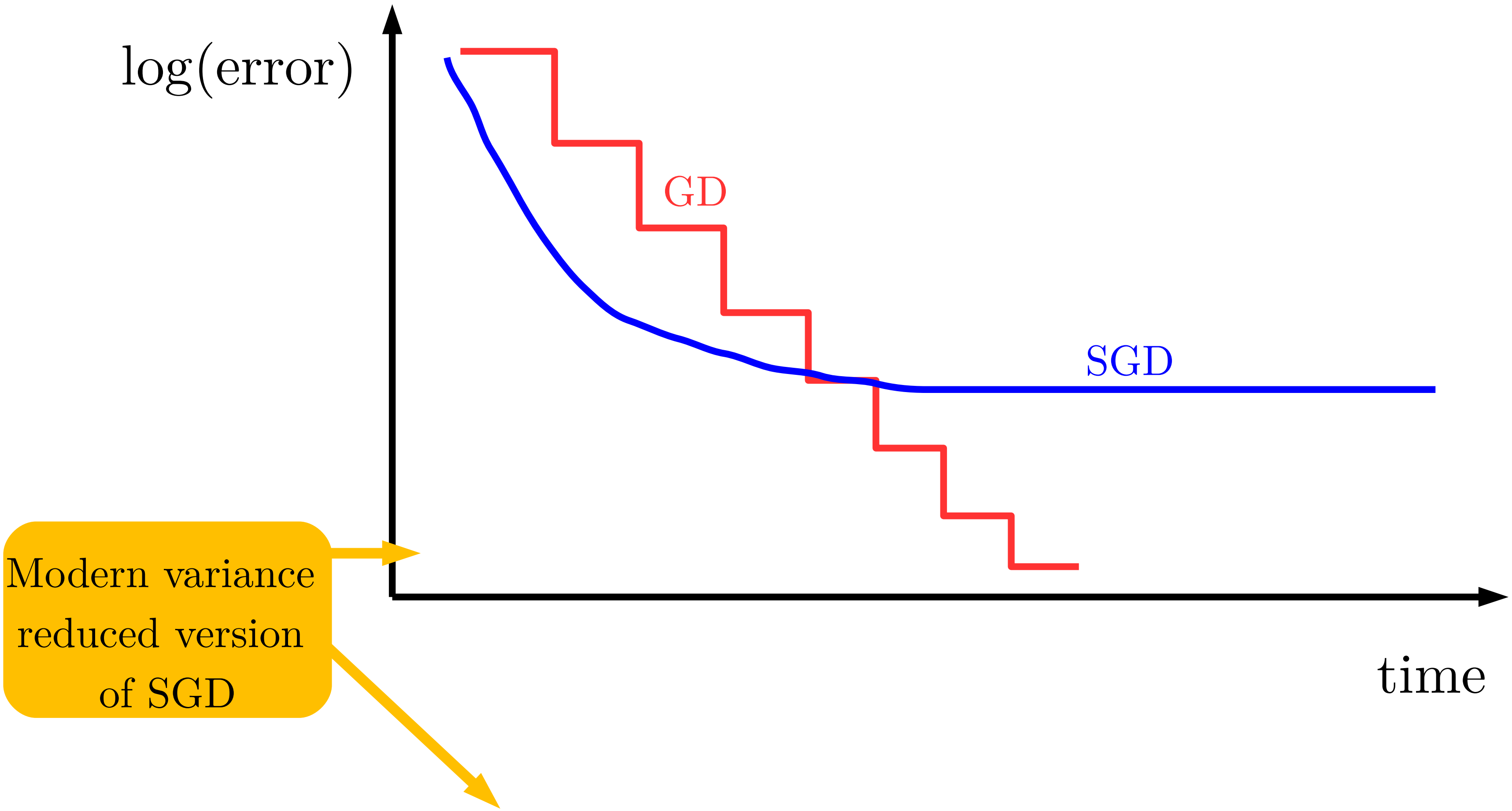

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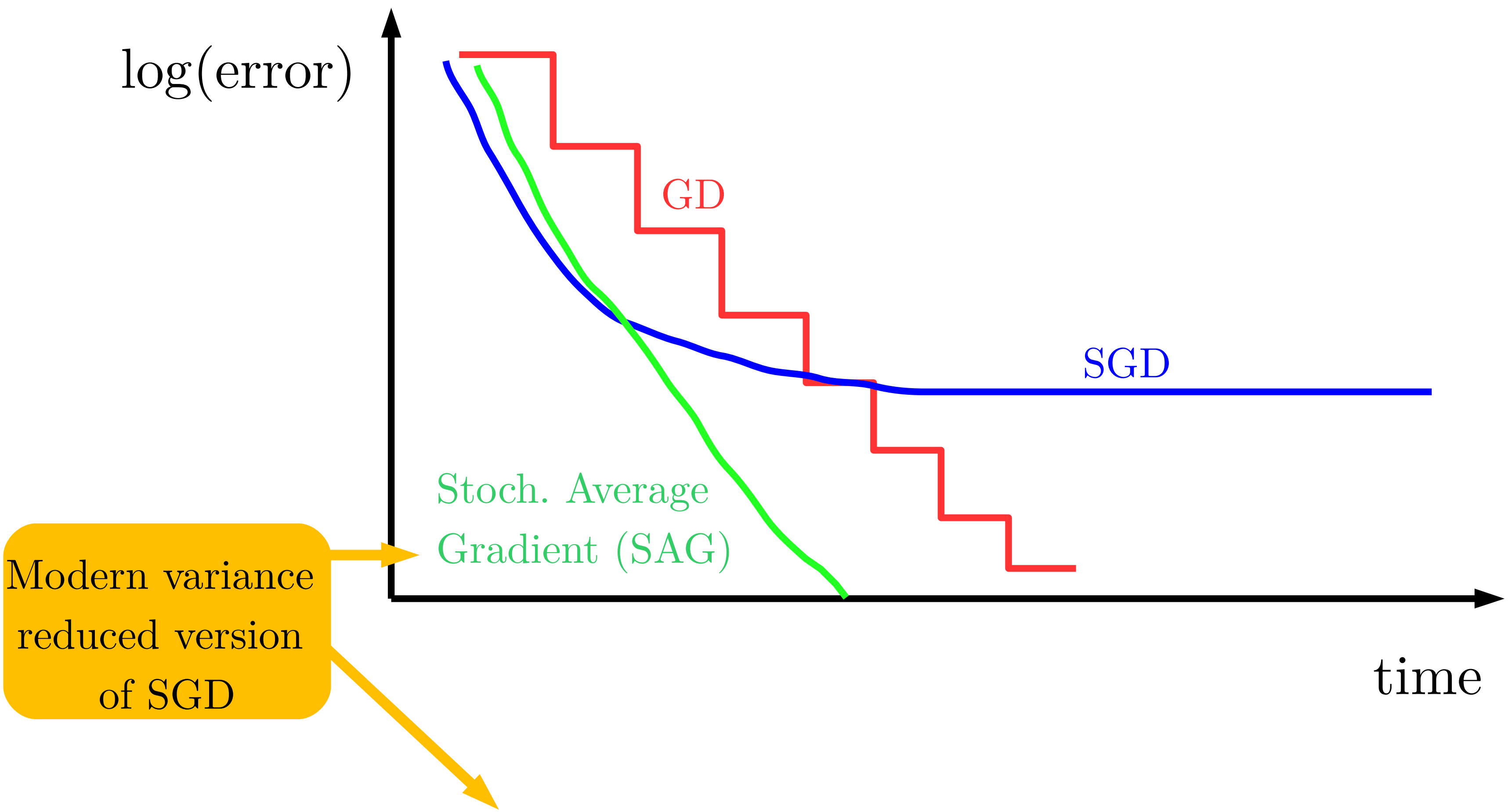

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20 min tea time break?

Practical SGD for Sparse Data

Lazy SGD updates for Sparse Data

L2 regularizor + linear hypothesis

Finite Sum Training Problem

$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} \ell\left(\langle w, x^i \rangle, y^i\right) + \frac{\lambda}{2} ||w||_2^2$$

Assume each data point x^i is s-sparse, how many operations does each SGD step cost?

Lazy SGD updates for Sparse Data

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$$\begin{aligned} w^{t+1} &= w^t - \alpha_t \left(\ell'(\langle w^t, x^i \rangle, y^i) x^i + \lambda w^t\right) \\ &= (1 - \lambda \alpha_t) w^t - \alpha_t \ell'(\langle w^t, x^i \rangle, y^i) x^i \end{aligned}$$

Lazy SGD updates for Sparse Data

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$$\begin{aligned} w^{t+1} &= w^t - \alpha_t \left(\ell'(\langle w^t, x^i \rangle, y^i) x^i + \lambda w^t\right) \\ &= \underbrace{(1 - \lambda \alpha_t) w^t}_{\text{Rescaling } O(d)} - \underbrace{\alpha_t \ell'(\langle w^t, x^i \rangle, y^i) x^i}_{\text{Addition sparse vector } O(s)} \end{aligned}$$

Rescaling $O(d)$ + Addition sparse vector $O(s)$ = $O(d)$

Lazy SGD updates for Sparse Data

SGD step

$$w^{t+1} = (1 - \lambda\alpha_t)w^t - \alpha_t \ell'(\langle w^t, x^i\rangle, y^i)x^i$$

EXE: re-write the iterates using $w^t = \beta_t z^t$ where $\beta_t \in \mathbb{R}$, $z^t \in \mathbb{R}^d$

Can you update β_t and z^t so that each iteration is $O(s)$?

Lazy SGD updates for Sparse Data

SGD step

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$$\begin{aligned}\beta_{t+1} z^{t+1} &= (1-\lambda\alpha_t)\beta_t z^t - \alpha_t \ell'(\beta_t\langle z^t, x^i\rangle, y^i)x^i \\ &= (1-\lambda\alpha_t)\beta_t \left(z^t - \frac{\alpha_t \ell'(\beta_t\langle z^t, x^i\rangle, y^i)}{(1-\lambda\alpha_t)\beta_t} x^i \right)\end{aligned}$$

Lazy SGD updates for Sparse Data

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$$\beta_{t+1} = (1-\lambda\alpha_t)\beta_t, \qquad z^{t+1} = z^t - \frac{\alpha_t \ell'(\beta_t\langle z^t, x^i\rangle, y^i)}{(1-\lambda\alpha_t)\beta_t} x^i$$

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$$\beta_{t+1}z^{t+1} = (1-\lambda\alpha_t)\beta_t z^t - \alpha_t \ell'(\beta_t\langle z^t, x^i\rangle, y^i)x^i$$

$$= \underbrace{(1-\lambda\alpha_t)\beta_t}_{\beta_{t+1}} \underbrace{\left(z^t - \frac{\alpha_t \ell'(\beta_t\langle z^t, x^i\rangle, y^i)}{(1-\lambda\alpha_t)\beta_t}x^i\right)}_{z^{t+1}}$$

$O(1)$ scaling +
$O(s)$ sparse add
$= O(s)$ update

$$\beta_{t+1} = (1-\lambda\alpha_t)\beta_t, \qquad z^{t+1} = z^t - \frac{\alpha_t \ell'(\beta_t\langle z^t, x^i\rangle, y^i)}{(1-\lambda\alpha_t)\beta_t}x^i$$

Momentum

Issue with Gradient Descent

Solving the *training problem*: $$\min_{w \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^{n} f_i(w) =: f(w)$$

Baseline method: Gradient Descent (GD)

$$w^{t+1} = w^t - \gamma \nabla f(w^t)$$

Step size/
Learning rate

Why GD and the the Issues

Local rate of change

$$\Delta(d) \;:=\; \lim_{s \to 0^+} \frac{f(x+ds) - f(x)}{s}$$

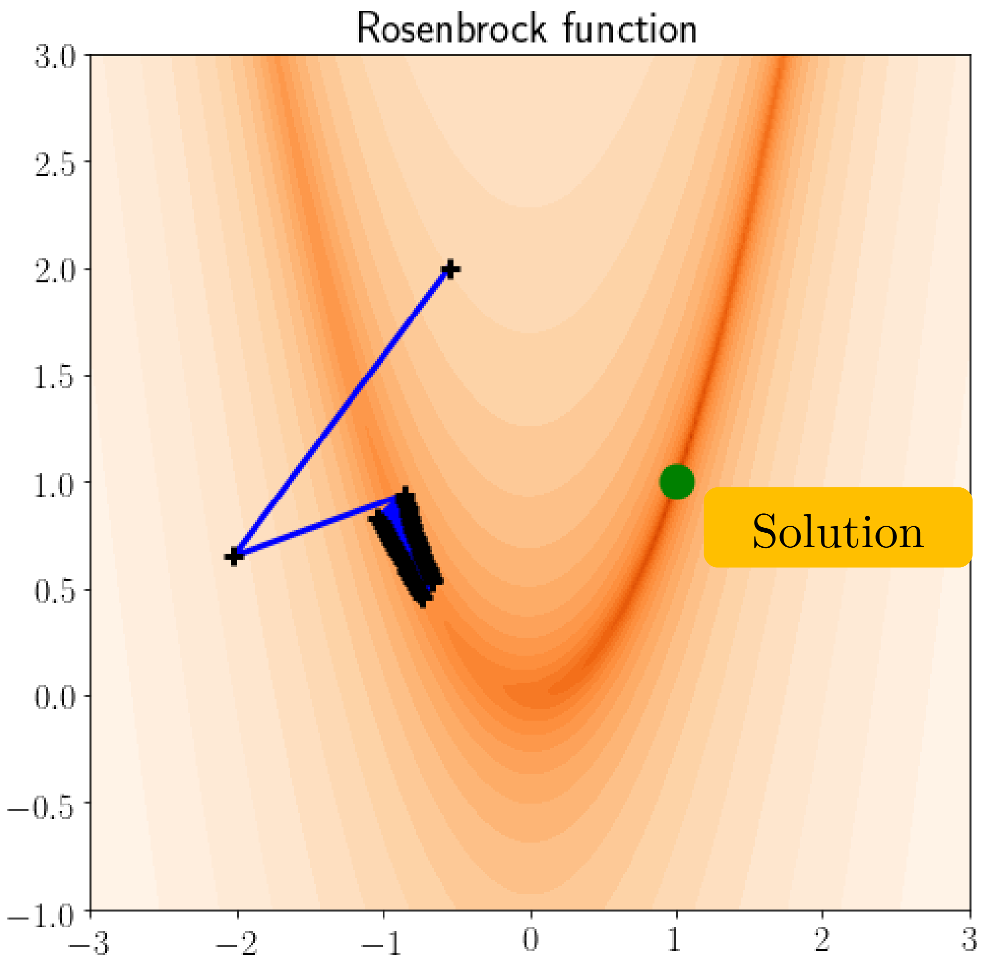
Max local rate

$$\frac{\nabla f(w^t)}{\|\nabla f(w^t)\|} \;:=\; \max_{w \in \mathbb{R}^d} \Delta(d)$$
$$\text{subject to} \quad \|d\| \;=\; 1$$

GD is the "steepest descent"

Issue with Gradient Descent

$$f(x_1, x_2) = 100(x_1 - x_2^2)^2 + (1 - x_2)^2$$



Get's stuck in "flat" valleys

Give momentum to keep going

Adding some Momentum to GD

Heavey Ball Method:

$$w^{t+1} = w^t - \gamma \nabla f(w^t) + \beta \underbrace{(w^t - w^{t-1})}_{\text{Adds ``Inertia'' to update}}$$

Adding some Momentum to GD

Heavey Ball Method:

$$w^{t+1} = w^t - \gamma \nabla f(w^t) + \underbrace{\beta(w^t - w^{t-1})}_{\text{Adds ``Inertia'' to update}}$$

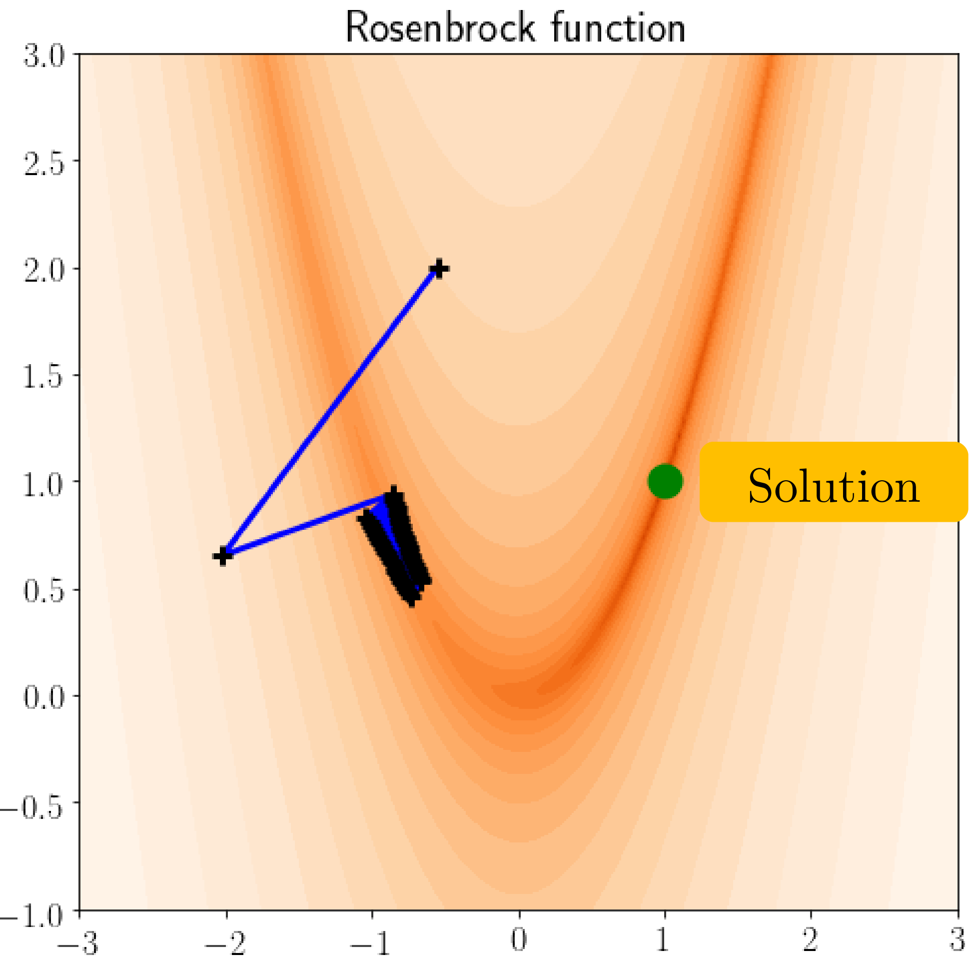
GD with momentum (GDm):

Adds "Momentum" to update

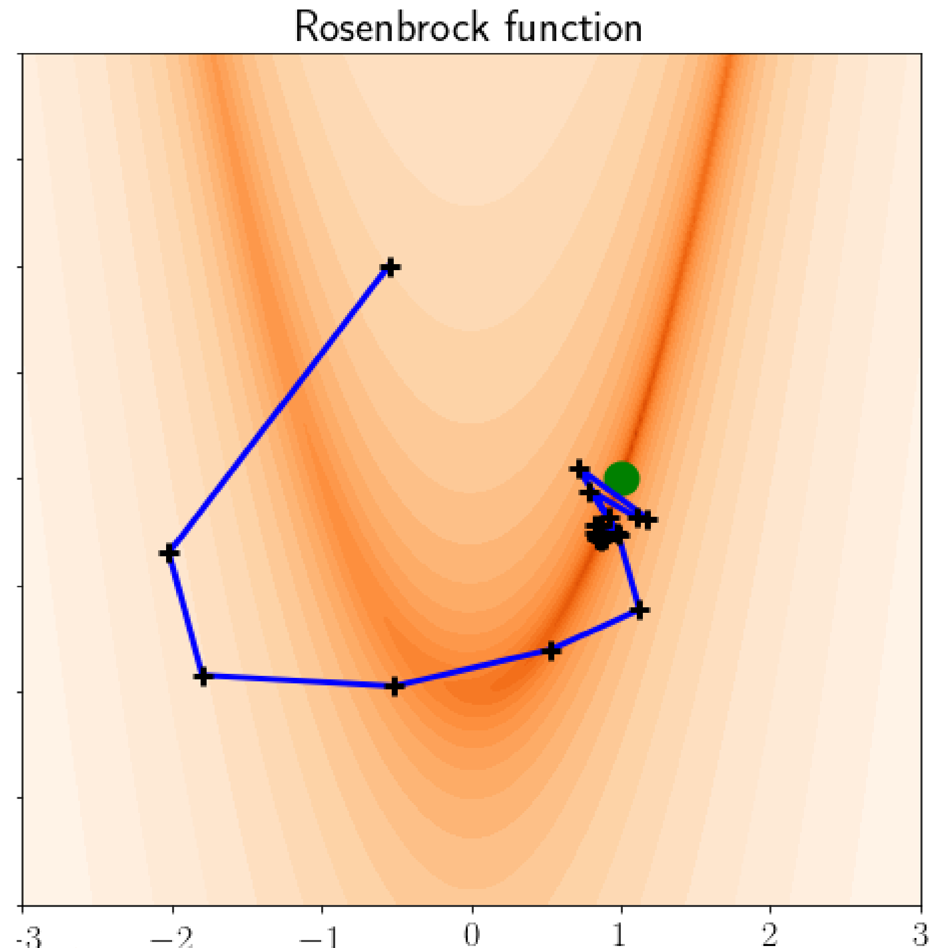
$$m^t = \beta\, m^{t-1} + \nabla f(w^t)$$

$$w^{t+1} = w^t - \gamma\, m^t$$

Issue with Gradient Descent



Solution



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Give momentum to keep going

GDm and Heavy Ball Equivalence

GD with momentum:

$$m^t = \beta\, m^{t-1} + \nabla f(w^t)$$

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$$\begin{aligned} w^{t+1} &= w^t - \gamma\, m^t \\ &= w^t - \gamma\,(\beta m^{t-1} + \nabla f(w^t)) \\ &= w^t - \gamma\, \nabla f(w^t) - \gamma\beta\, m^{t-1} \\ &= w^t - \gamma\, \nabla f(w^t) + \frac{\gamma\beta}{\gamma}\,(w^t - w^{t-1}) \end{aligned}$$

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Heavey Ball Method:

$$w^{t+1} = w^t - \gamma\, \nabla f(w^t) + \beta(w^t - w^{t-1})$$

Convergence of Gradient Descent with Momentum

Polyak 1964

Theorem Let f be μ–strongly convex and L–smooth, that is

stepsize

$$\mu I \quad \preceq \quad \nabla^2 f(w) \quad \preceq \quad LI, \quad \forall w \in \mathbb{R}^d$$

If $\gamma = \dfrac{4}{(\sqrt{L}+\sqrt{\mu})^2}$ and $\beta = \dfrac{\sqrt{L}-\sqrt{\mu}}{\sqrt{L}+\sqrt{\mu}}$ then SGDm converges

momentum parameter

$$\Rightarrow \quad \|w^t - w^*\| \;\leq\; \left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^t \|w^0 - w^*\|$$

$\kappa := L/\mu$

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$$\|w^t - w^*\| \;\leq\; \left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^t \|w^0 - w^*\|$$

$\kappa := L/\mu$

Corollary $t \;\geq\; \dfrac{\sqrt{\kappa}+1}{2}\log\left(\dfrac{1}{\epsilon}\right) \;\Rightarrow\; \dfrac{\|w^t - w^*\|}{\|w^0 - w^*\|} \leq \epsilon$

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momentum parameter

$$\Rightarrow \quad \|w^t - w^*\| \leq \left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^t \|w^0 - w^*\|$$

Compare with $\kappa \log(1/\epsilon)$ of GD

$\kappa := L/\mu$

Corollary $t \geq \dfrac{\sqrt{\kappa}+1}{2} \log\left(\dfrac{1}{\epsilon}\right) \quad \Rightarrow \quad \dfrac{\|w^t - w^*\|}{\|w^0 - w^*\|} \leq \epsilon$

Proof sketch: GDm convergence

Fundamental Theorem of Calculus

$$\int_{s=0}^{1} \nabla^2 f(\underbrace{w_s}_{w_s := w^* + s(w^t - w^*)}) ds (w^t - w^*) = \nabla f(w^t) - \nabla f(w^*) = \nabla f(w^t)$$

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w^{t+1} - w^* &= w^t - w^* - \gamma \nabla f(w^t) + \beta(w^t - w^{t-1}) \\
&= \left(I - \gamma \int_{s=0}^{1} \nabla^2 f(w^s)\right)(w^t - w^*) + \beta(w^t - \overbrace{w^{t-1}}^{+w^* - w^*}) \\
&= \left((1+\beta)I - \gamma \int_{s=0}^{1} \nabla^2 f(w^s)\right)(w^t - w^*) - \beta(w^{t-1} - w^*)
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Depends on past. Difficult recurrence

Proof: Convergence of Heavy Ball

$$z^{t+1} = \begin{bmatrix} w^{t+1} - w^* \\ w^t - w^* \end{bmatrix} \in \mathbb{R}^{2d}$$

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EXE on Eigenvalues:

$$\text{If } \gamma = \frac{4}{(\sqrt{L}+\sqrt{\mu})^2} \text{ and } \quad \beta = \frac{\sqrt{L}-\sqrt{\mu}}{\sqrt{L}+\sqrt{\mu}} \text{ then}$$

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Adding Momentum to SGD

Rumelhart, Hinton, Geoffrey, Ronald, 1986, Nature

Stochastic Heavey Ball Method:

$$w^{t+1} = w^t - \gamma \nabla f_{j_t}(w^t) + \beta\underbrace{(w^t - w^{t-1})}_{\text{Adds ``Inertia'' to update}}$$

Sampled i.i.d
$j \in \{1, \ldots, n\}$
$j \sim \frac{1}{n}$

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SGD with momentum (SGDm):

$$m^t = \beta\, m^{t-1} + \nabla f_{j_t}(w^t)$$

$$w^{t+1} = w^t - \gamma\, m^t$$

SGDm and Averaging

$$
\begin{aligned}
m^t &= \beta\, m^{t-1} + \nabla f_{j_t}(w^t) \\
&= \beta\, m^{t-2} + \nabla f_{j_t}(w^t) + \beta \nabla f_{j_{t-1}}(w^{t-1}) \\
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http://fa.bianp.net/teaching/2018/COMP-652/stochastic_gradient.html

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Acts like an approximate variance reduction since

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$$\sum_{i=1}^{t} \beta^i \nabla f_{j_{t-i}}(w^{t-i}) \approx \sum_{i=1}^{n} \frac{1}{n} \nabla f_i(w^t) = \nabla f(w^t)$$

http://fa.bianp.net/teaching/2018/COMP-652/stochastic_gradient.html

Why Machine Learners Like SGD

Why Machine Learners like SGD

Though we solve:

$$\min_{w\in\mathbf{R}^d} \frac{1}{n}\sum_{i=1}^{n} \ell\left(h_w(x^i), y^i\right) + \lambda R(w)$$

We want to solve:

The statistical learning problem:

Minimize the expected loss over an *unknown* expectation

$$\min_{w\in\mathbf{R}^d} \mathbb{E}_{(x,y)\sim\mathcal{D}}\left[\ell\left(h_w(x), y\right)\right]$$

SGD can solve the statistical learning problem!

Why Machine Learners like SGD

The statistical learning problem:

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SGD ∞.0 for learning

Set $w^0 = 0$, $\alpha > 0$

for $t = 0, 1, 2, \ldots, T-1$

sample $(x, y) \sim \mathcal{D}$

calculate $v_t \in \partial \ell(h_{w^t}(x), y)$

$w^{t+1} = w^t - \alpha v_t$

Output $\overline{w}^T = \frac{1}{T}\sum_{t=1}^{T} w^t$

Bring laptops for Thursday TD !

RMG, Nicolas Loizou, Xun Qian, Alibek Sailanbayev, Egor Shulgin and Peter Richtárik (2019), ICML
SGD: general analysis and improved rates

RMG, P. Richtarik, F. Bach (2018), preprint online
Stochastic quasi-gradient methods: Variance reduction via Jacobian sketching

N. Gazagnadou, RMG, J. Salmon (2019) , ICML 2019.
Optimal mini-batch and step sizes for SAGA

O. Sebbouh, N. Gazagnadou, S. Jelassi, F. Bach, RMG
Neurips 2019, preprint online. **Towards closing the gap between the theory and practice of SVRG**