Optimization for Data Science

Stochastic Gradient Methods

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Solving the Finite Sum Training Problem

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!

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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 $\{1, \ldots, n\}$ 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

SGD 0.0 Constant stepsize

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

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

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

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

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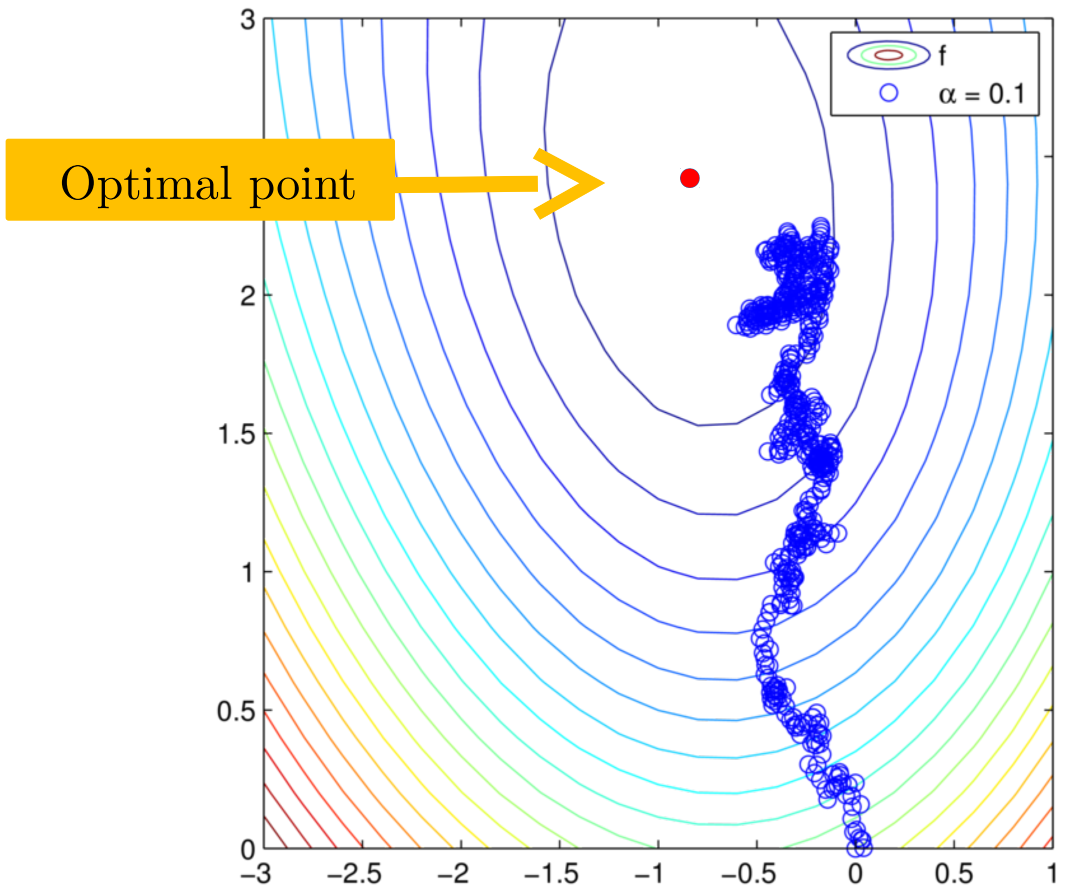
Stochastic Gradient Descent



Assumptions for Convergence

Strong Convexity

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

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

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

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Expected Bounded Stochastic Gradients

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

Complexity / Convergence

Theorem

If $\frac{1}{\lambda} \geq \alpha > 0$ then the iterates of the SGD method satisfy

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

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

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

Shows that $\alpha \approx 0$

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

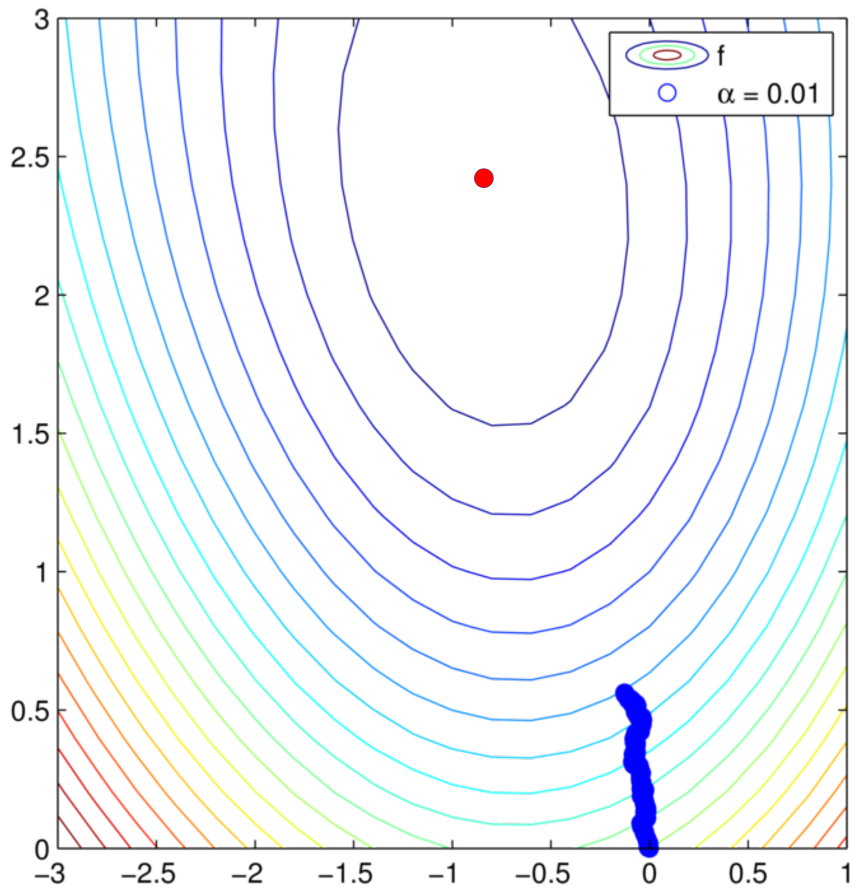
$$\begin{aligned} \mathbb{E} \left[||w^{t+1} - w^*||_2^2 \right] &\leq (1 - \alpha\lambda) \mathbb{E} \left[||w^t - w^*||_2^2 \right] + \alpha^2 B^2 \\ &= (1 - \alpha\lambda)^{t+1} ||w^0 - w^*||_2^2 + \textstyle\sum_{i=0}^t (1 - \alpha\lambda)^i \alpha^2 B^2 \end{aligned}$$

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

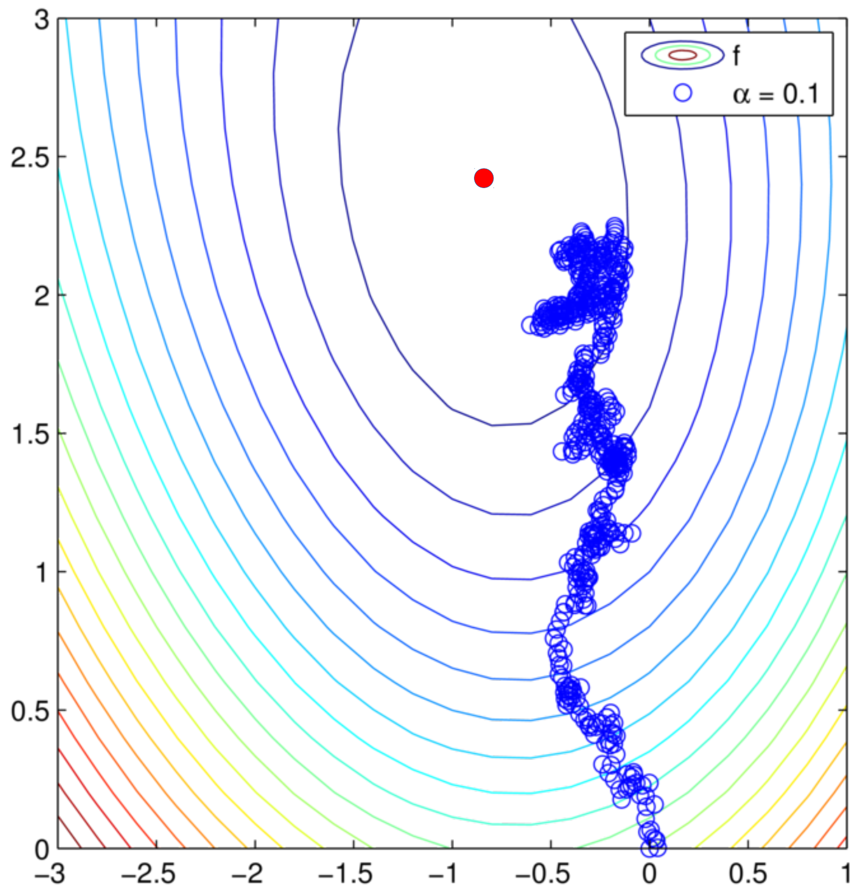
$$\mathbb{E} \left[||w^{t+1} - w^*||_2^2 \right] \leq (1 - \alpha\lambda)^{t+1} ||w^0 - w^*||_2^2 + \tfrac{\alpha}{\lambda} B^2$$

Stochastic Gradient Descent

α =0.01

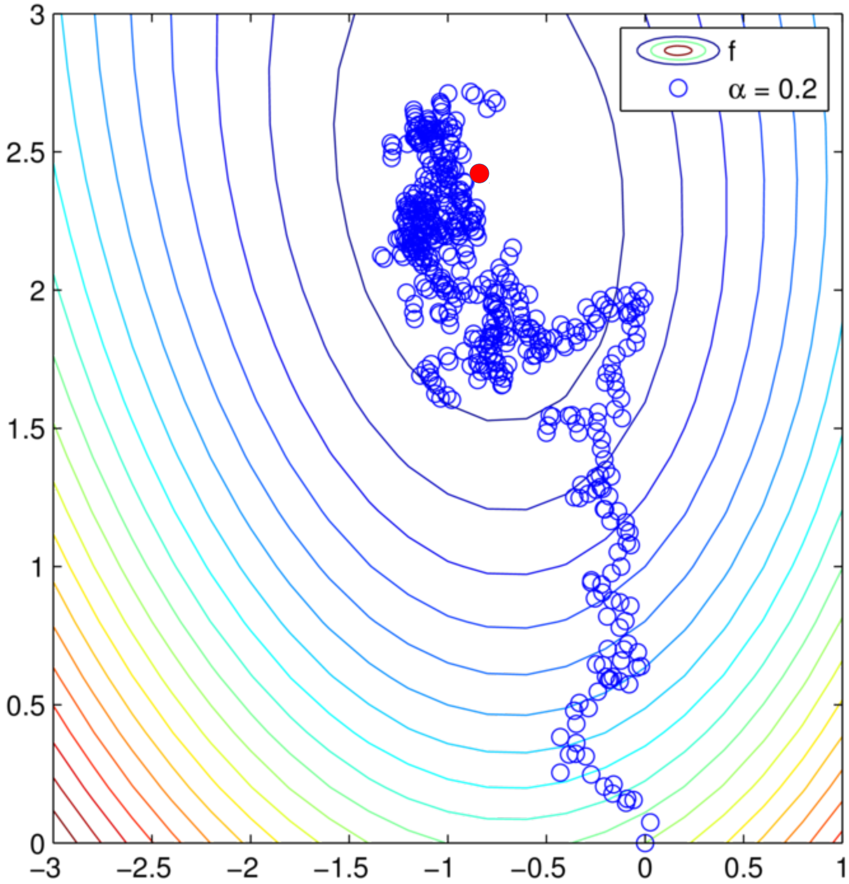


Stochastic Gradient Descent
α =0.1

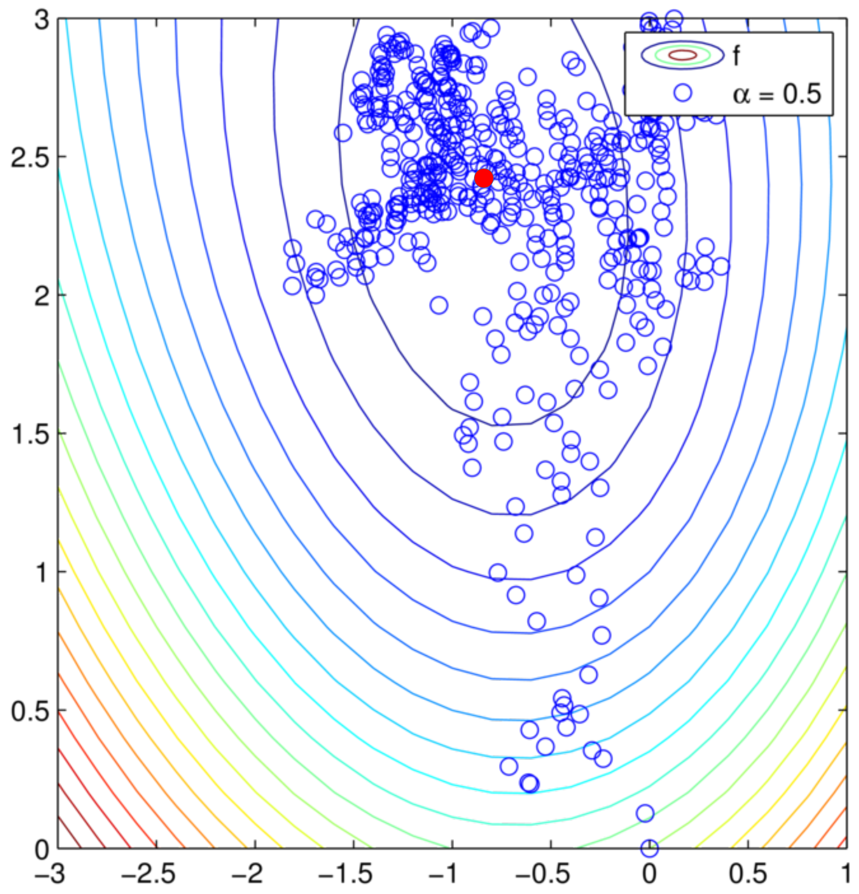


Stochastic Gradient Descent

α =0.2

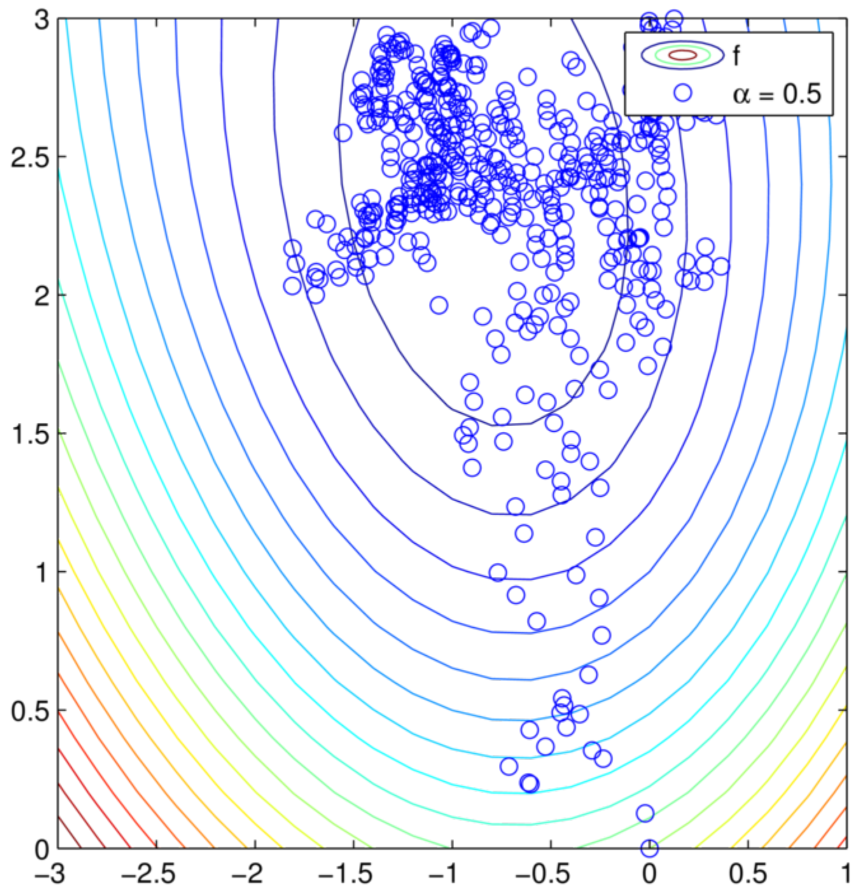


Stochastic Gradient Descent
α =0.5



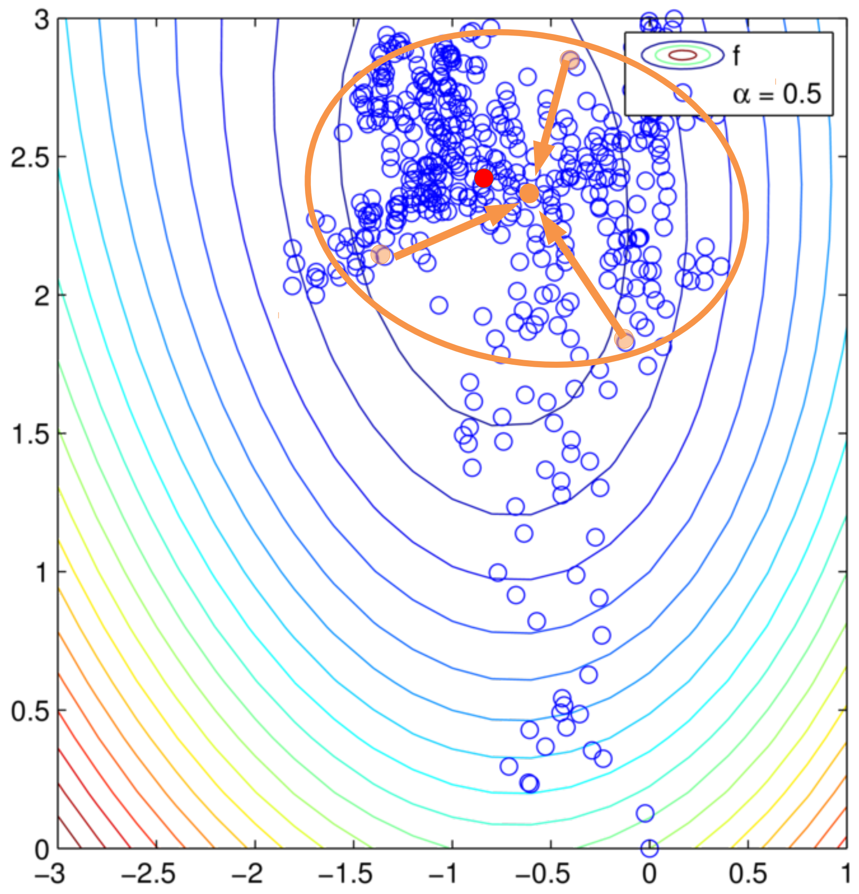
Stochastic Gradient Descent

α =0.5



1) Start with big steps and end with smaller steps

Stochastic Gradient Descent
α =0.5



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 $\alpha_0 > 0$, $\alpha_t = \frac{\alpha_0}{\sqrt{t+1}}$,

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

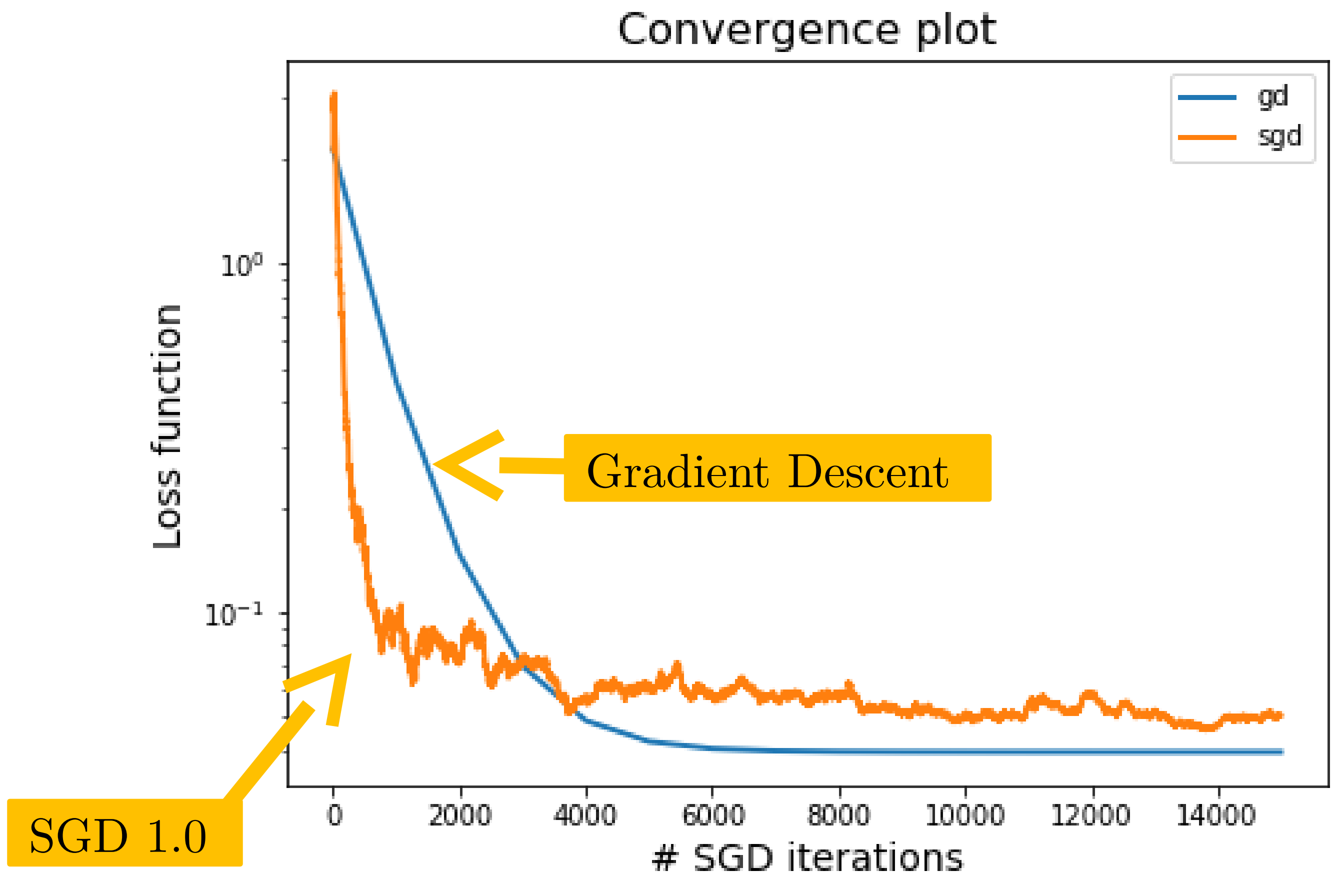
Shrinking Stepsize

How should we sample j ?

Why is $\alpha_t \sim \dfrac{1}{\sqrt{t}}$?

Does this converge?

SGD with shrinking stepsize
Compared with Gradient Descent



SGD with shrinking stepsize
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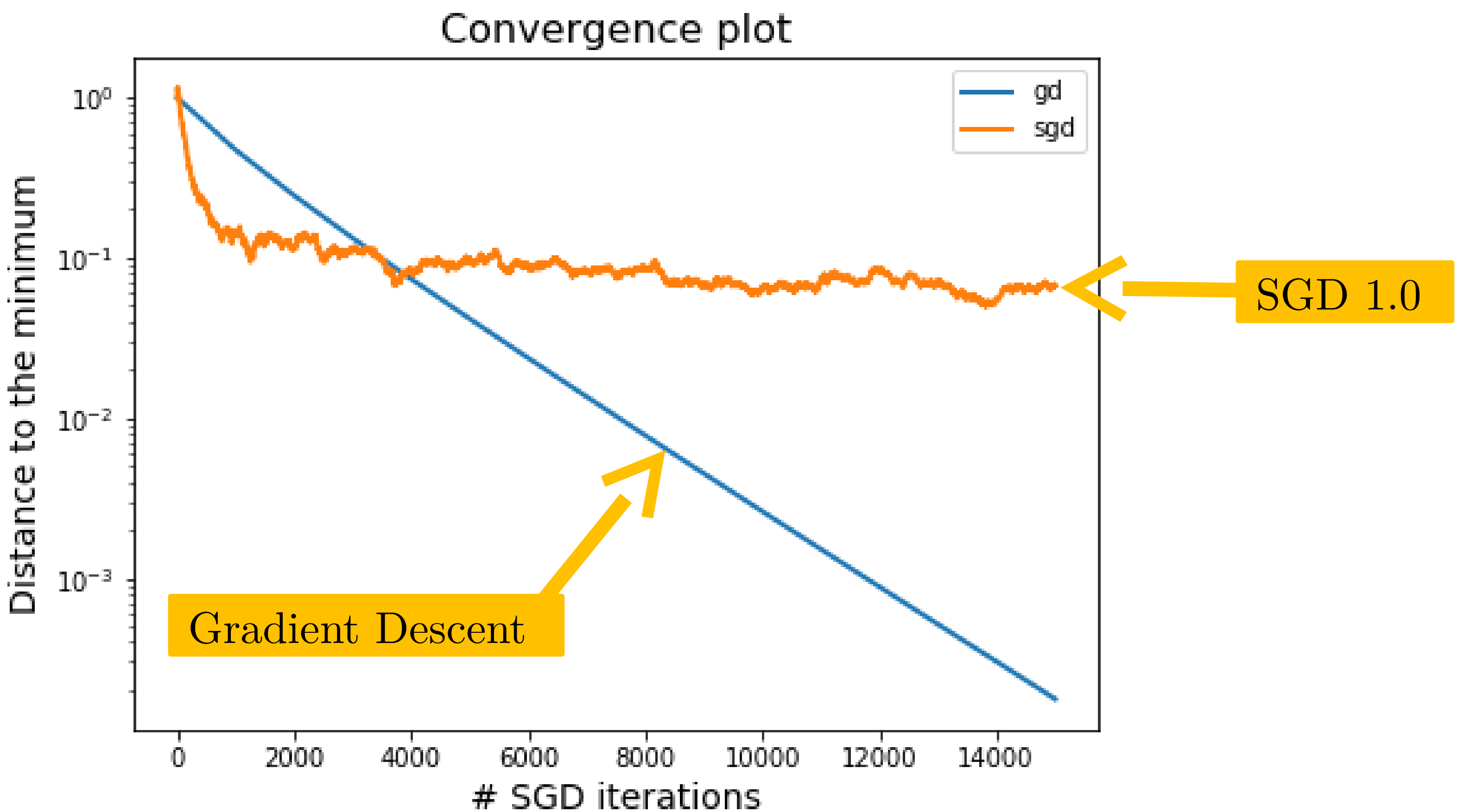

SGD Theory

Assumptions

- $f(w)$ is convex
- Subgradients bounded $\mathbb{E}_j||\nabla f_j(w^t)||_2 \leq B$
- There exists $r \in \mathbb{R}_+$ such that $w^* \in D := \{w \ : \ ||w|| \leq r\}$

SGD 1.1 theoretical

Set $w^1 = 0$, $\alpha_t \in \mathbb{R}_+$, $\alpha_t \underset{t\to\infty}{\rightarrow} 0$

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

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

  $w^{t+1} = \mathrm{proj}_D\left(w^t - \alpha_t \nabla f_j(w^t)\right)$

Output w^T

Convergence for Convex

Theorem (Shrinking stepsize)

If $f(w)$ is convex,

and $\alpha_t = \dfrac{\alpha_0}{\sqrt{t}}$ then SGD1.1 satisfies

$$\mathbb{E}[f(w^T)] - f(w^*) = O\left(\frac{1}{\sqrt{T}}\right)$$

Ohad Shamir and Tong Zhang (2013)
International Conference on Machine Learning
Stochastic Gradient Descent for Non-smooth Optimization: Convergence Results and Optimal Averaging Schemes.

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Sublinear convergence

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Complexity for Strong. Convex

Theorem (Shrinking stepsize)

If $f(w)$ is λ–strongly convex,

and $\alpha_t = \dfrac{\alpha_0}{\lambda t}$ then SGD1.1 satisfies

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Faster
Sublinear
convergence

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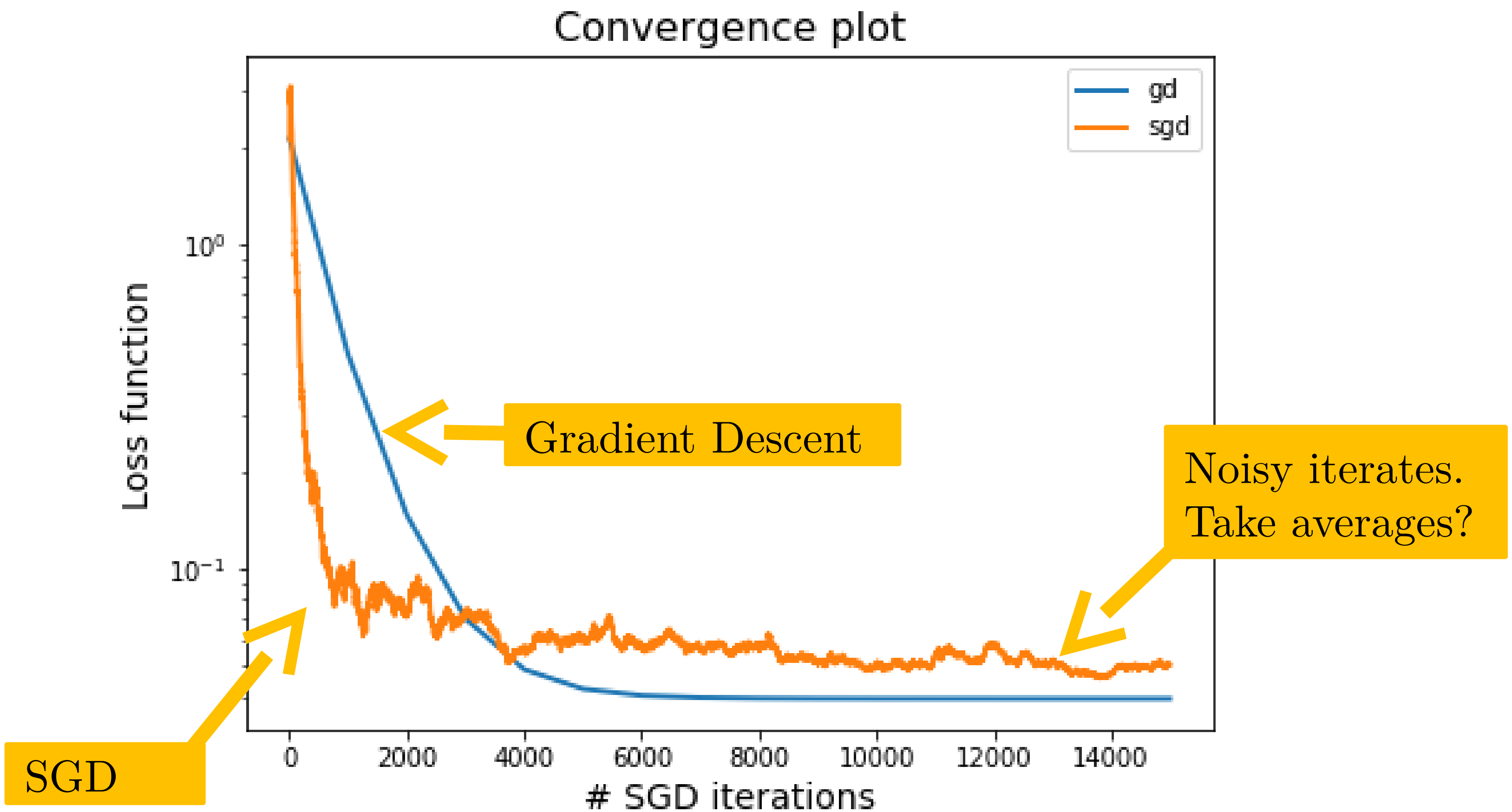
Stochastic Gradient Descent

Compared with Gradient Descent



Complexity for Convex SGDA

Theorem for SGD 1.1 (Shrinking stepsize)

Let $\overline{w}^T = \frac{1}{T}\sum_{t=1}^T w^t, D = \{w : ||w|| \leq r\}$ and $r \in \mathbb{R}_+$

such that $||w^*||_2 \leq r$. If $\alpha_t = \dfrac{2r}{B\sqrt{t}}$ then

$$\mathbb{E}[f(\overline{w}^T)] - f(w^*) \leq \frac{3rB}{\sqrt{T}}$$

SGDA 1.1 for Convex

Set $w^1 = 0$, $\alpha_t = \frac{2r}{B\sqrt{t}}$,

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

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

  $w^{t+1} = \mathrm{proj}_D\left(w^t - \alpha_t \nabla f_j(w^t)\right)$

Output $\overline{w}^T$

Complexity for Convex SGDA

Theorem for SGD 1.1 (Shrinking stepsize)

Let $\overline{w}^T = \frac{1}{T}\sum_{t=1}^T w^t$, $D = \{w : ||w|| \leq r\}$ and $r \in \mathbb{R}_+$ such that $||w^*||_2 \leq r$. If $\alpha_t = \dfrac{2r}{B\sqrt{t}}$ then

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Sublinear convergence

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Proof Part I:

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

Taking expectation with respect to j

Unbiased estimator

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

Convexity

Bounded Stoch grad

Taking total expectation and re-arranging

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

Summing up for *1* to T

$$
\begin{aligned}
\textstyle\sum_{t=1}^T \left(\mathbb{E}\left[f(w^t)\right] - f(w^*)\right) &\leq \frac{1}{2\alpha_1}||w^1 - w^*||_2^2 + \frac{1}{2}\sum_{t=1}^{T-1}\left(\frac{1}{\alpha_{t+1}} - \frac{1}{\alpha_t}\right)\mathbb{E}\left[||w^t - w^*||_2^2\right] \\
&\quad - \frac{1}{2\alpha_{T+1}}\mathbb{E}\left[||w^{T+1} - w^*||_2^2\right] + \frac{B^2}{2}\sum_{t=1}^T \alpha_t
\end{aligned}
$$

Proof Part II:

$$\sum_{t=1}^{T}(\mathbb{E}\left[f(w^t)\right] - f(w^*)) \quad \leq \quad \frac{1}{2\alpha_1}||w^1 - w^*||_2^2 + \frac{1}{2}\sum_{t=1}^{T-1}\left(\frac{1}{\alpha_{t+1}} - \frac{1}{\alpha_t}\right)\mathbb{E}\left[||w^t - w^*||_2^2\right]$$
$$-\frac{1}{2\alpha_{T+1}}\mathbb{E}\left[||w^{T+1} - w^*||_2^2\right] + \frac{B^2}{2}\sum_{t=1}^{T}\alpha_t$$

$||w||_2^2 \;\leq\; r^2$
$\alpha_{t+1} \;\leq\; \alpha_t$

$$\leq \quad \frac{2r^2}{\alpha_1} + 2r^2\sum_{t=1}^{T-1}\left(\frac{1}{\alpha_{t+1}} - \frac{1}{\alpha_t}\right) + \frac{B^2}{2}\sum_{t=1}^{T}\alpha_t$$

$$= \quad \frac{2r^2}{\alpha_T} + \frac{B^2}{2}\sum_{t=1}^{T}\alpha_t$$

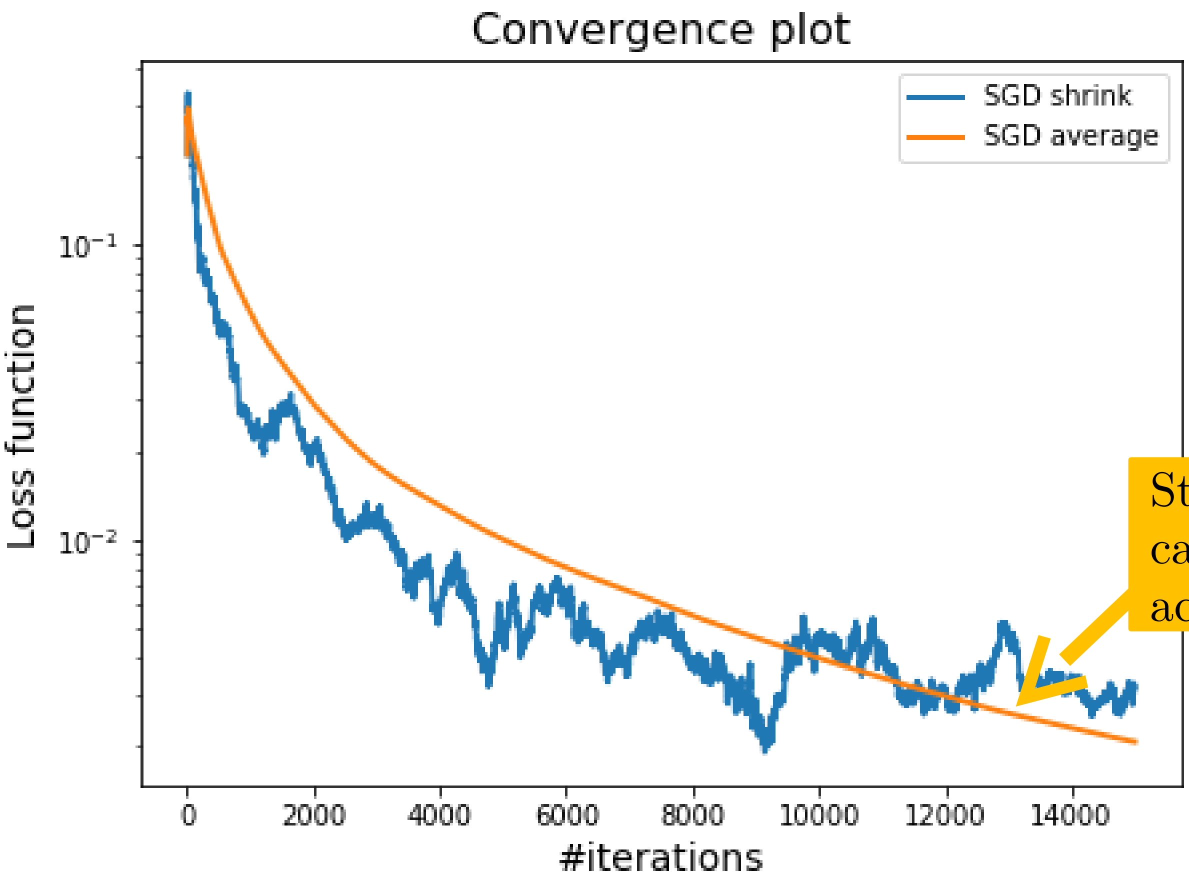
Finally let $\overline{w}^T = \frac{1}{T}\sum_{t=1}^{T} w^t$ and dividing by T, using $\alpha_t = \frac{\alpha_0}{\sqrt{t}}$

$$\mathbb{E}[f(\bar{w}_T)] - f(w^*)) \quad \leq \quad \frac{1}{T}\sum_{t=1}^{T}\mathbb{E}[f(w_t)] - f(w^*)) \leq \frac{r^2\sqrt{T}}{T\alpha_0} + \frac{B^2}{2T}\sum_{t=1}^{T}\frac{\alpha_0}{\sqrt{t}}$$
$$\leq \quad \frac{1}{\sqrt{T}}\left(\frac{2r^2}{\alpha_0} + \alpha_0 B^2\right)$$

Minimizing in α_0 gives $\alpha_0 = \sqrt{2}r/B$ and thus

$$\mathbb{E}[f(\bar{w}_T)] - f(w^*)) \quad \leq \quad \frac{1}{\sqrt{T}}\left(\sqrt{2}rB + \sqrt{2}rB\right) \leq \frac{3rB}{\sqrt{T}}$$

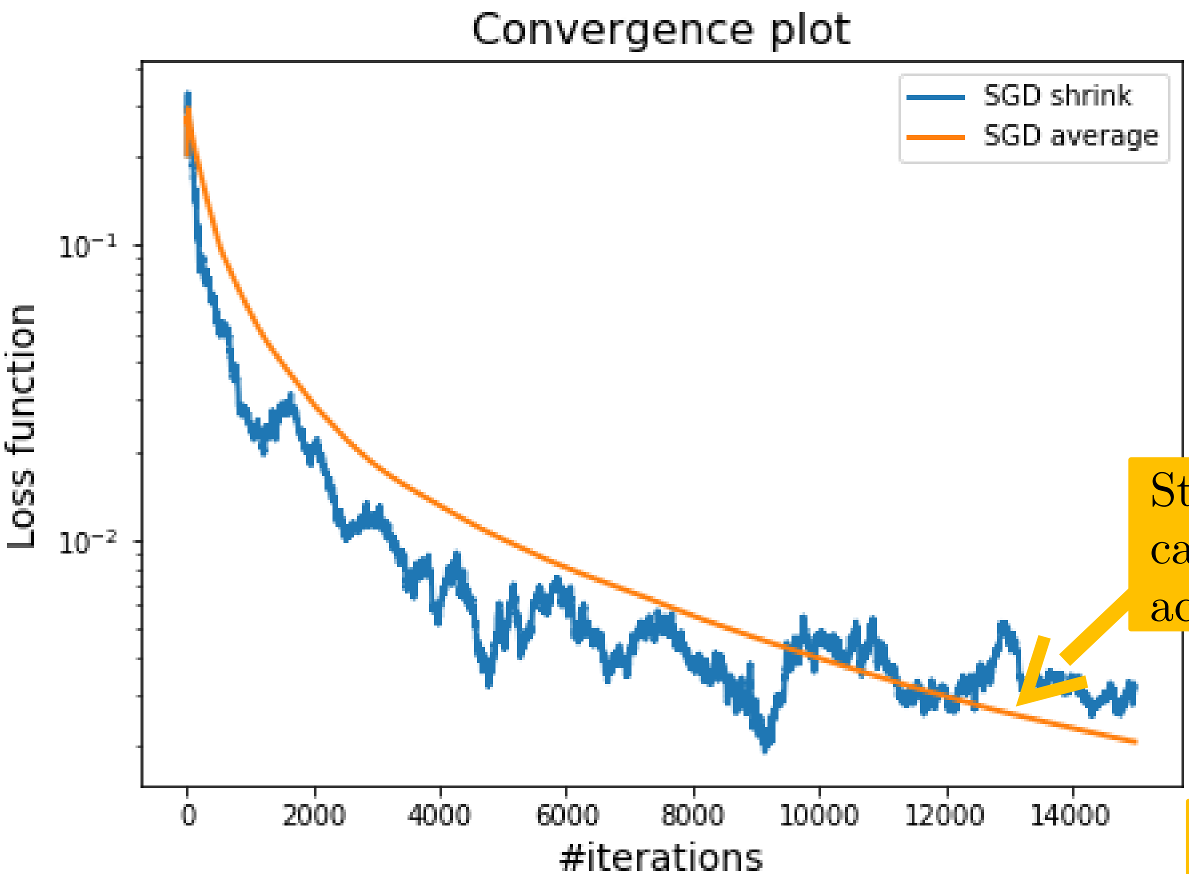
Stochastic Gradient Descent
With and without averaging



Starts slow, but can reach higher accuracy

Stochastic Gradient Descent

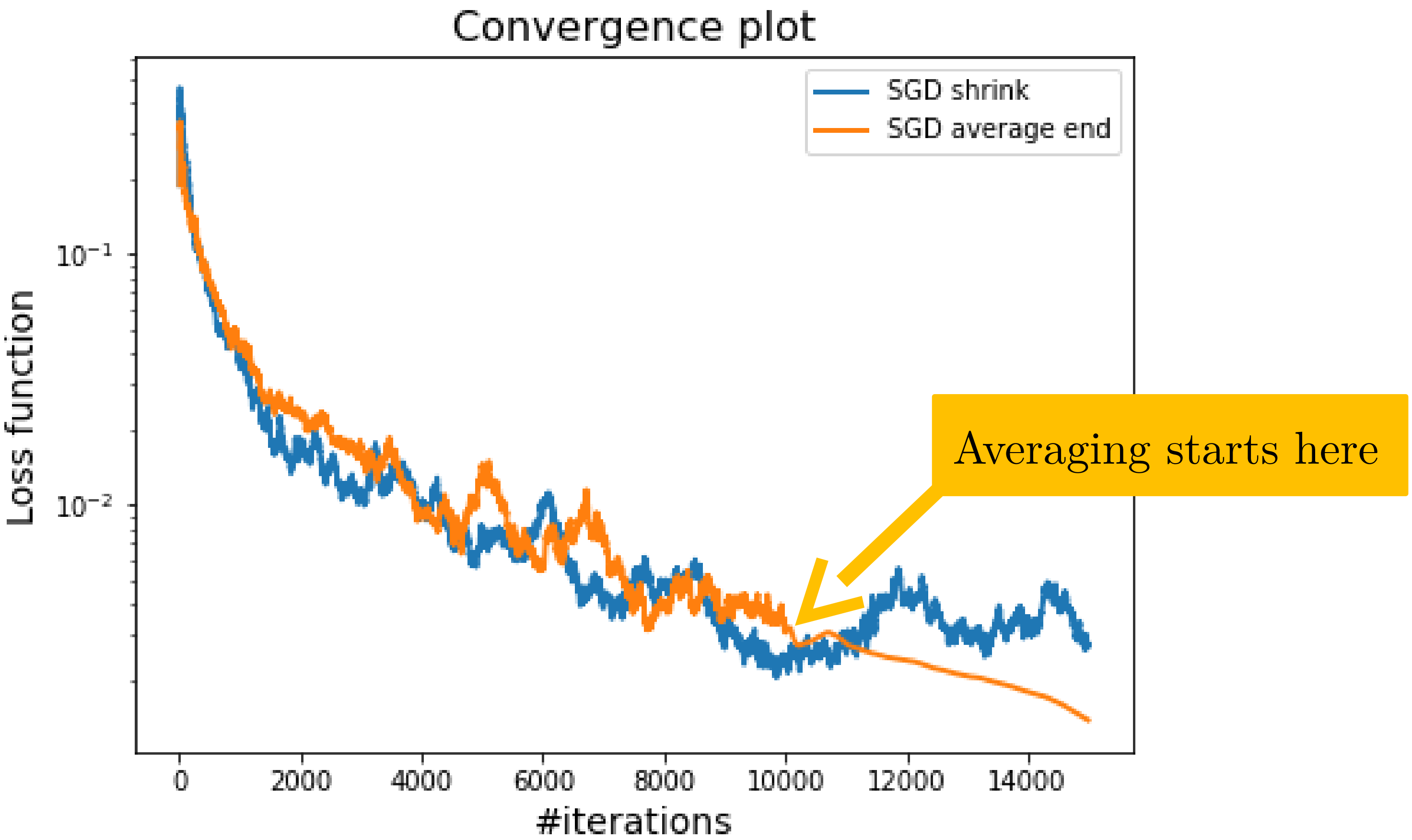
With and without averaging



Starts slow, but can reach higher accuracy

Only use averaging towards the end?

Stochastic Gradient Descent
Averaging the last iterates



Comparison GD and SGD for strongly convex

Approximate solution

$$\mathbb{E}[f(w^T)] - f(w^*) \leq \epsilon$$

$T \quad \geq$

SGD

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

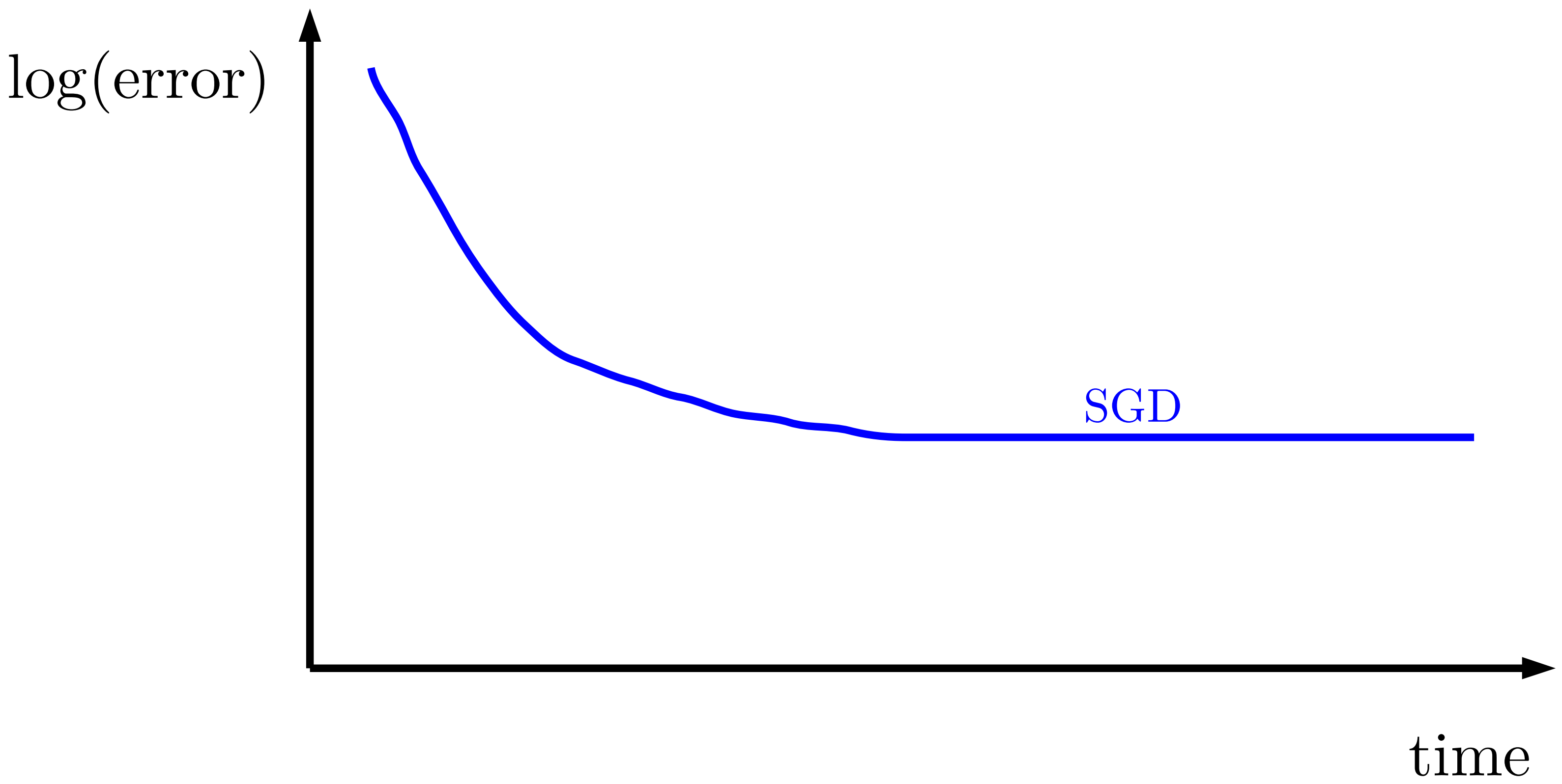
Gradient descent

$$O\left(\frac{nL}{\lambda}\log\left(\frac{1}{\epsilon}\right)\right)$$

What happens if ϵ is small?

What happens if n is big?

Comparison SGD vs GD



M. Schmidt, N. Le Roux, F. Bach (2016)
Mathematical Programming
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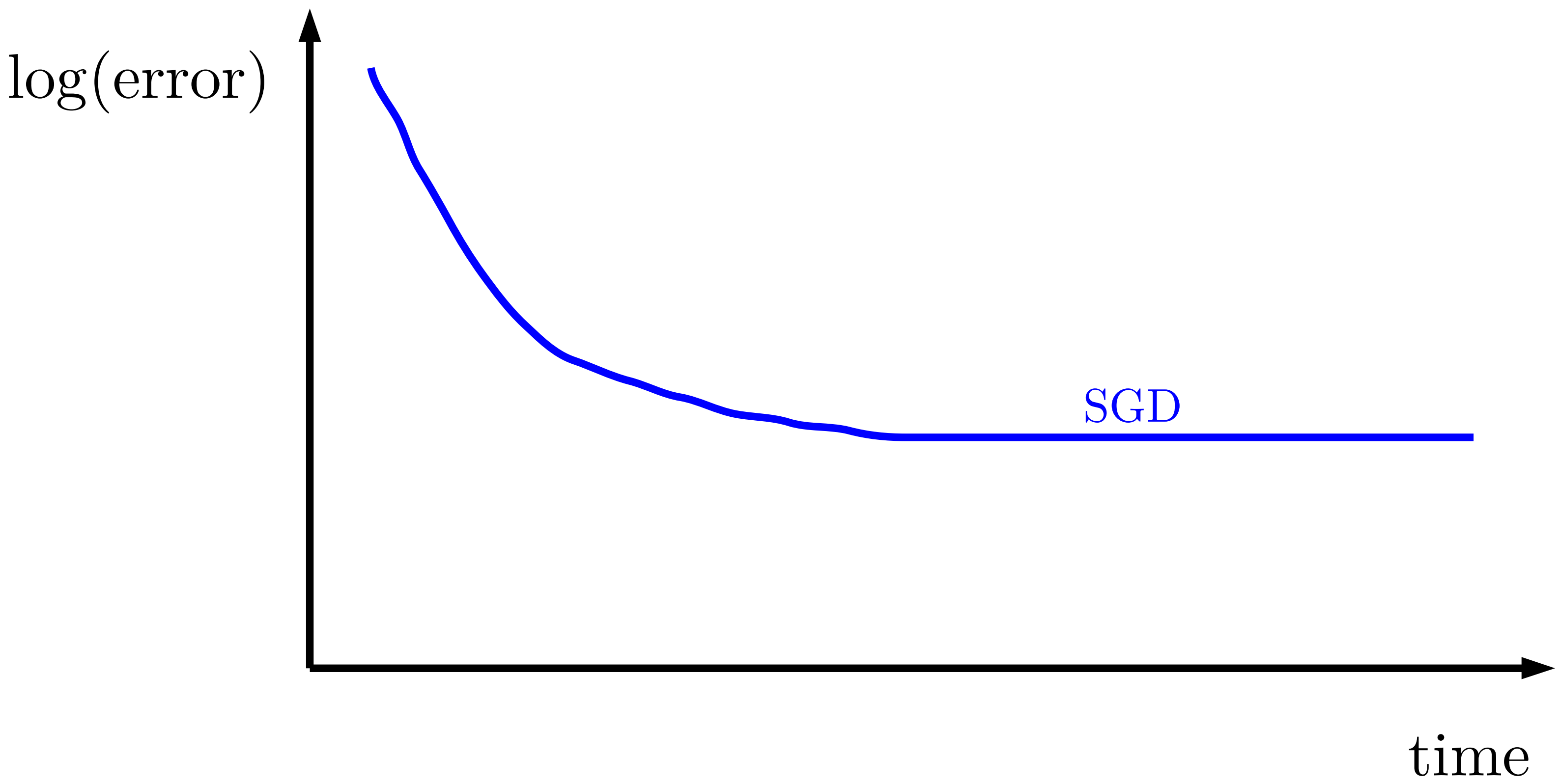
Comparison SGD vs GD



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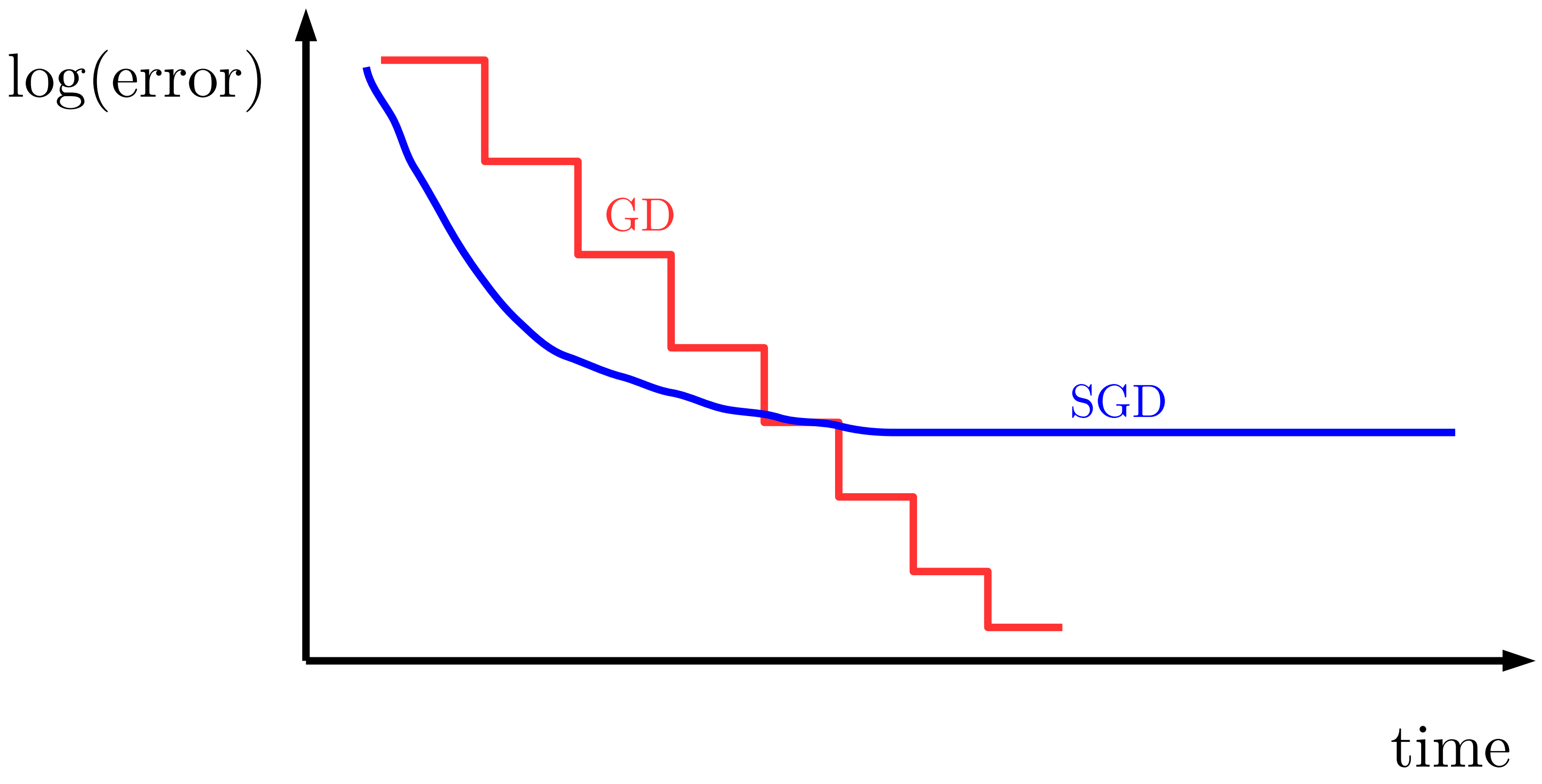

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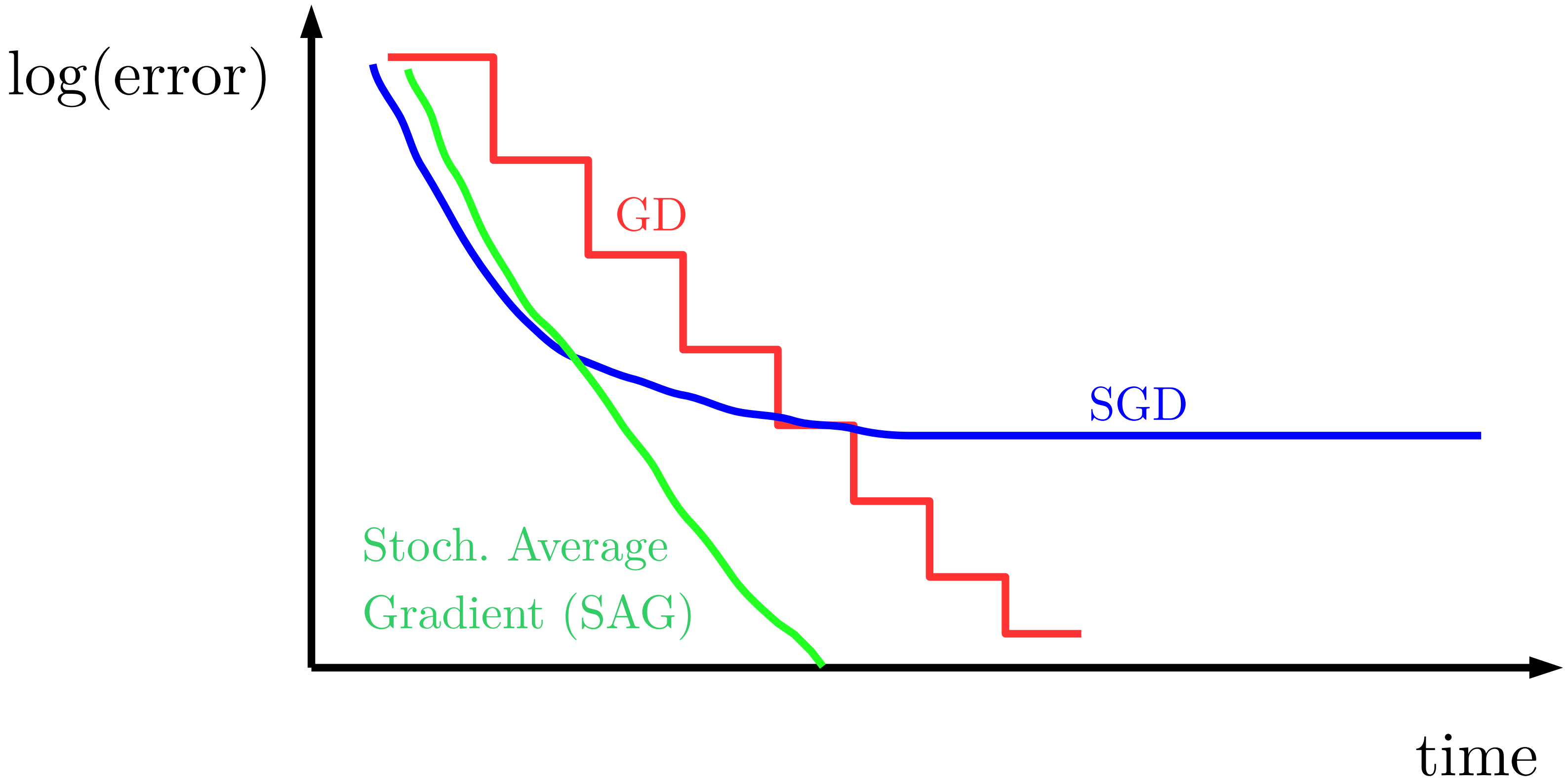

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Practical SGD for Sparse Data

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

Finite Sum Training Problem

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

L2 regularizor + linear hypothesis

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

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

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?

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

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 $O(s)$?

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

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

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

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Why Machine Learners Like SGD

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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!

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

Coding time!

Complexity for strongly convex

Theorem (Shrinking stepsize)

If $f(w)$ is λ–strongly convex, $\overline{w}^T = \dfrac{2}{T(T+1)} \displaystyle\sum_{t=0}^{T-1} t w^t$

and $\alpha_t = \dfrac{2}{\lambda(t+1)}$ then SGD1.2 satisfies

$$\mathbb{E}[f(\overline{w}^T)] - f(w^*) \leq \frac{2B^2}{\lambda(T+1)}$$

SGD 1.2 for Strongly Convex

Set $w^0 = 0$, $\alpha_t = \frac{2}{\lambda(t+1)}$,

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

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

$w^{t+1} = \mathrm{proj}_D\left(w^t - \alpha_t \nabla f_j(w^t)\right)$

Output $\overline{w}^T$

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Faster Sublinear convergence

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