Stochastic Gradient Methods

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Solving the Finite Sum Training Problem

Recap

Training Problem

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

General methods

$$\min f(w)$$

- Gradient Descent
- Quasi-Newton
- Conjugate Gradients

Two parts

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

- ISTA
- 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

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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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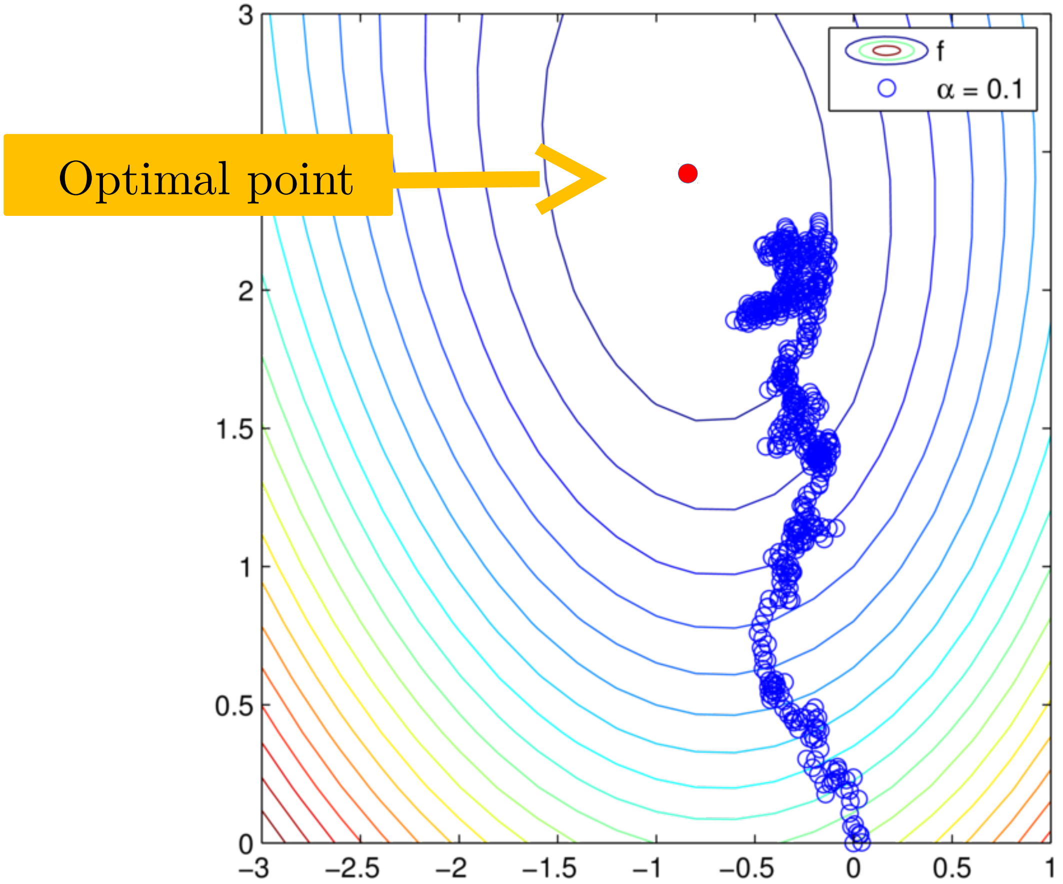
Stochastic Gradient Descent



Assumptions for Convergence

Strong Convexity

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

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

EXE: Using that

$$\frac{\sigma_{\min}(A)^2}{2}||w - y||_2^2 \leq \frac{1}{2}||A(w - y)||_2^2$$

Show that

$$\frac{1}{2}||Aw - b||_2^2 \geq \frac{1}{2}||Ay - b||_2^2 + \langle A^\top (Ay - b), w - y \rangle + \frac{\sigma_{\min}(A)^2}{2}||w - y||_2^2$$

Assumptions for Convergence

Often the same as the regularization parameter

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Strong convexity parameter!

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Expected Bounded Stochastic Gradients

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

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

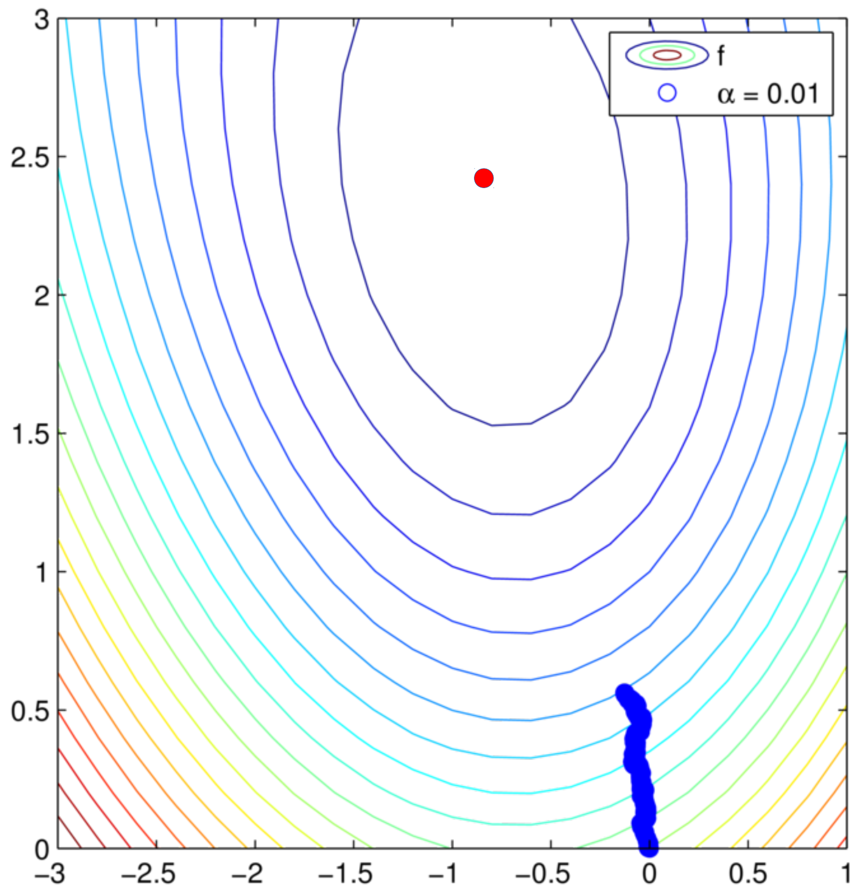
Taking total expectation

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

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

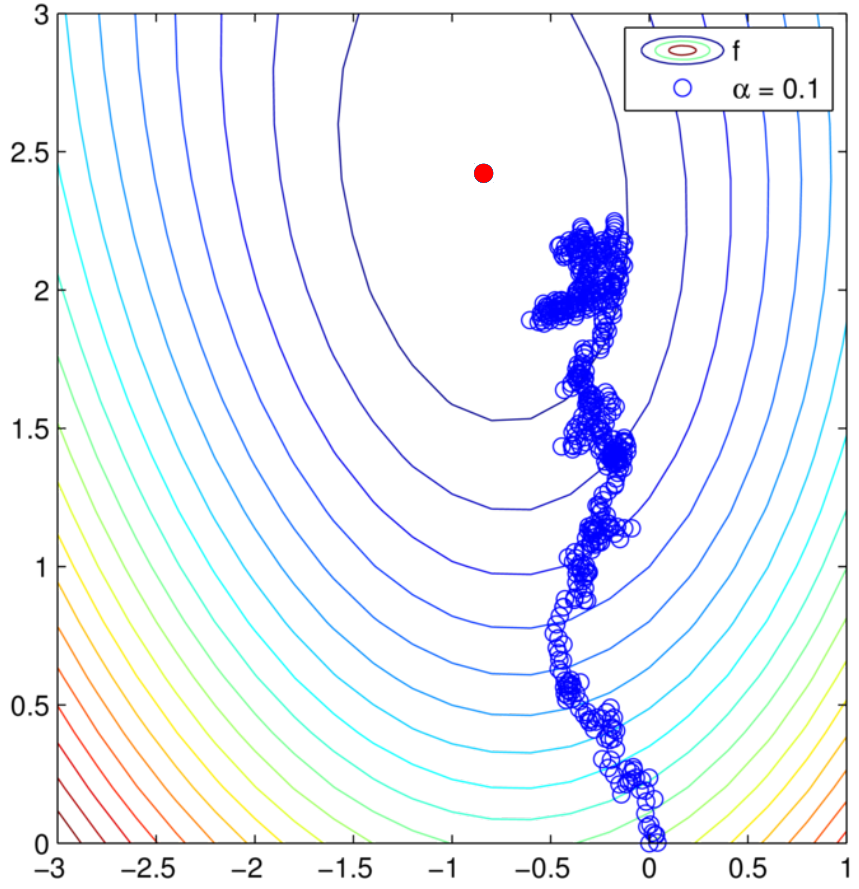
$$
\mathbb{E} \left[||w^{t+1} - w^*||_2^2 \right] \leq (1 - \alpha\lambda)^{t+1} ||w^0 - w^*||_2^2 + \tfrac{\alpha}{\lambda} B^2
$$

Stochastic Gradient Descent
α =0.01



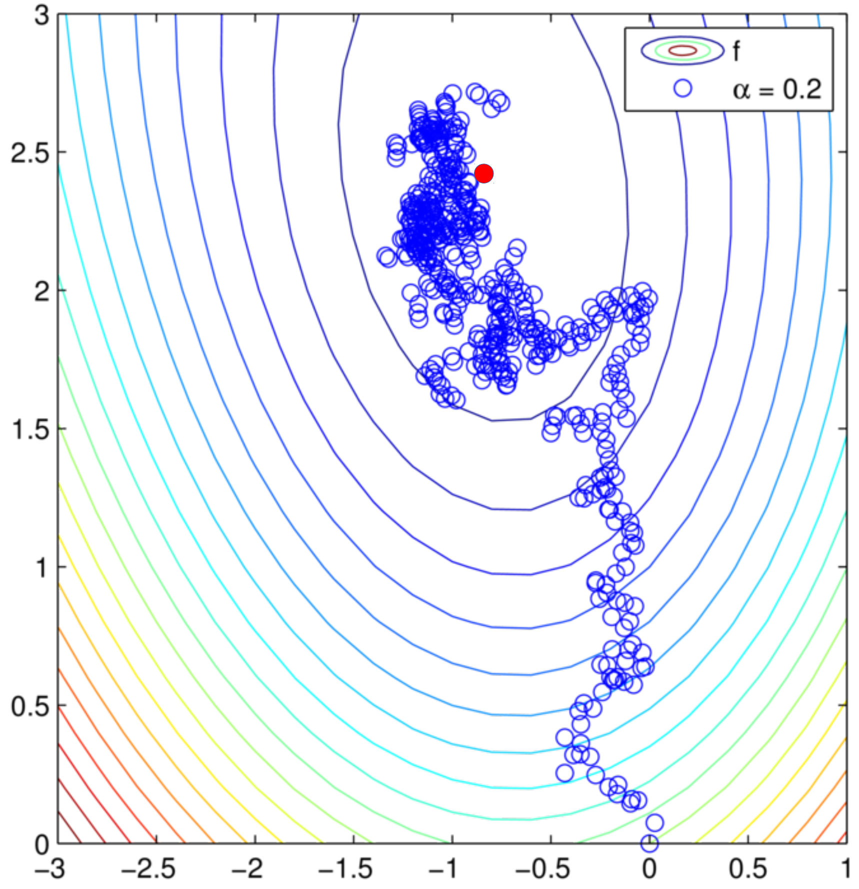
Stochastic Gradient Descent

$\alpha = 0.1$

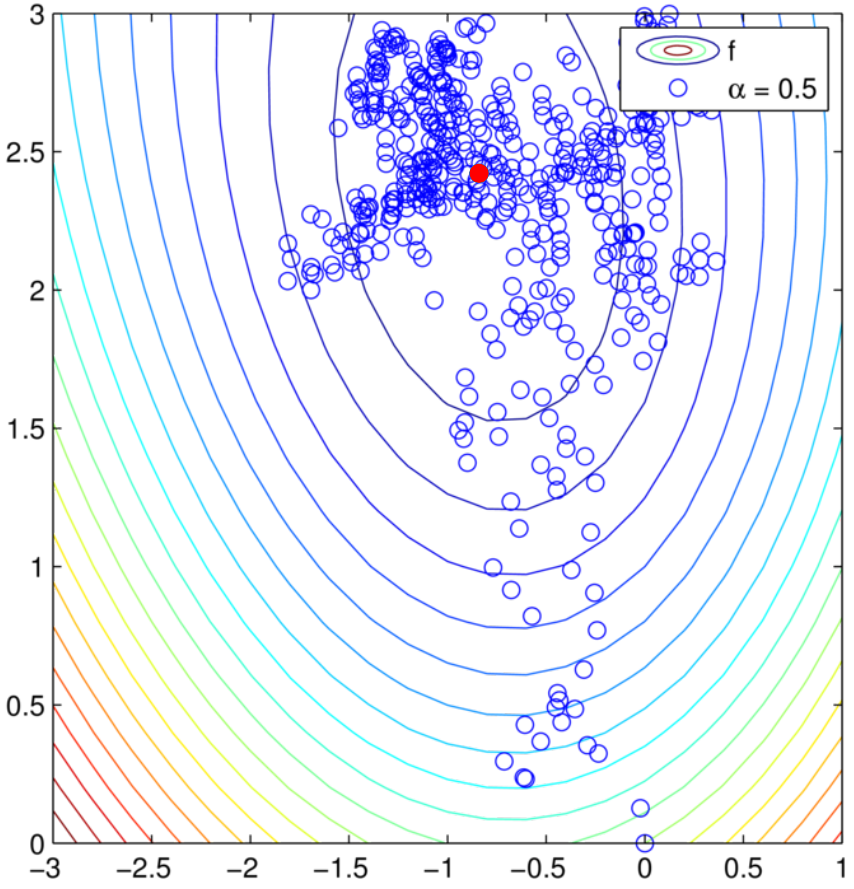


Stochastic Gradient Descent

α =0.2



Stochastic Gradient Descent
α =0.5



SGD shrinking stepsize

SGD 1.0: Descreasing stepsize

Set $w^0 = 0$, choose $\alpha > 0$, $\alpha_t = \frac{\alpha}{\sqrt{t+1}}$,

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 Theoretical Properties

Convergence for Convex

- $f(w)$ is convex
- Subgradients bounded

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

Convergence for Strongly Convex

- $f(w)$ is λ - strongly convex
- Subgradients bounded

$$\alpha_t = O\left(\frac{1}{\lambda t}\right) \quad \Rightarrow \quad \mathbb{E}[f(w^T)] - f(w^*) = O\left(\frac{1}{\lambda T}\right)$$

Complexity for Convex

Theorem for SGD 1.1 (Shrinking stepsize)

Let $D = \{x \,:\, ||x|| \leq r\}$ and $r \in \mathbb{R}_+$

such that $||w^*||_2 \leq r$. If $\alpha_t = \dfrac{\alpha}{\sqrt{t+1}}$ for $\alpha > 0$ then

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

SGD 1.1 for Convex

Set $w^0 = 0$, $\alpha > 0$, $\alpha_t = \frac{\alpha}{\sqrt{t+1}}$,
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 w^T

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Let $D = \{x \, : \, ||x|| \leq r\}$ and $r \in \mathbb{R}_+$

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Sublinear convergence

SGD 1.1 for Convex

Set $w^0 = 0, \ \alpha > 0, \ \alpha_t = \frac{\alpha}{\sqrt{t+1}},$

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

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

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

Output w^T

Complexity for Strong. Convex

Theorem (Shrinking stepsize)

If $f(w)$ is λ–strongly convex,

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

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

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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Faster
Sublinear
convergence

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Comparison GD and SGD for strongly convex

Approximate solution

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

SGD

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

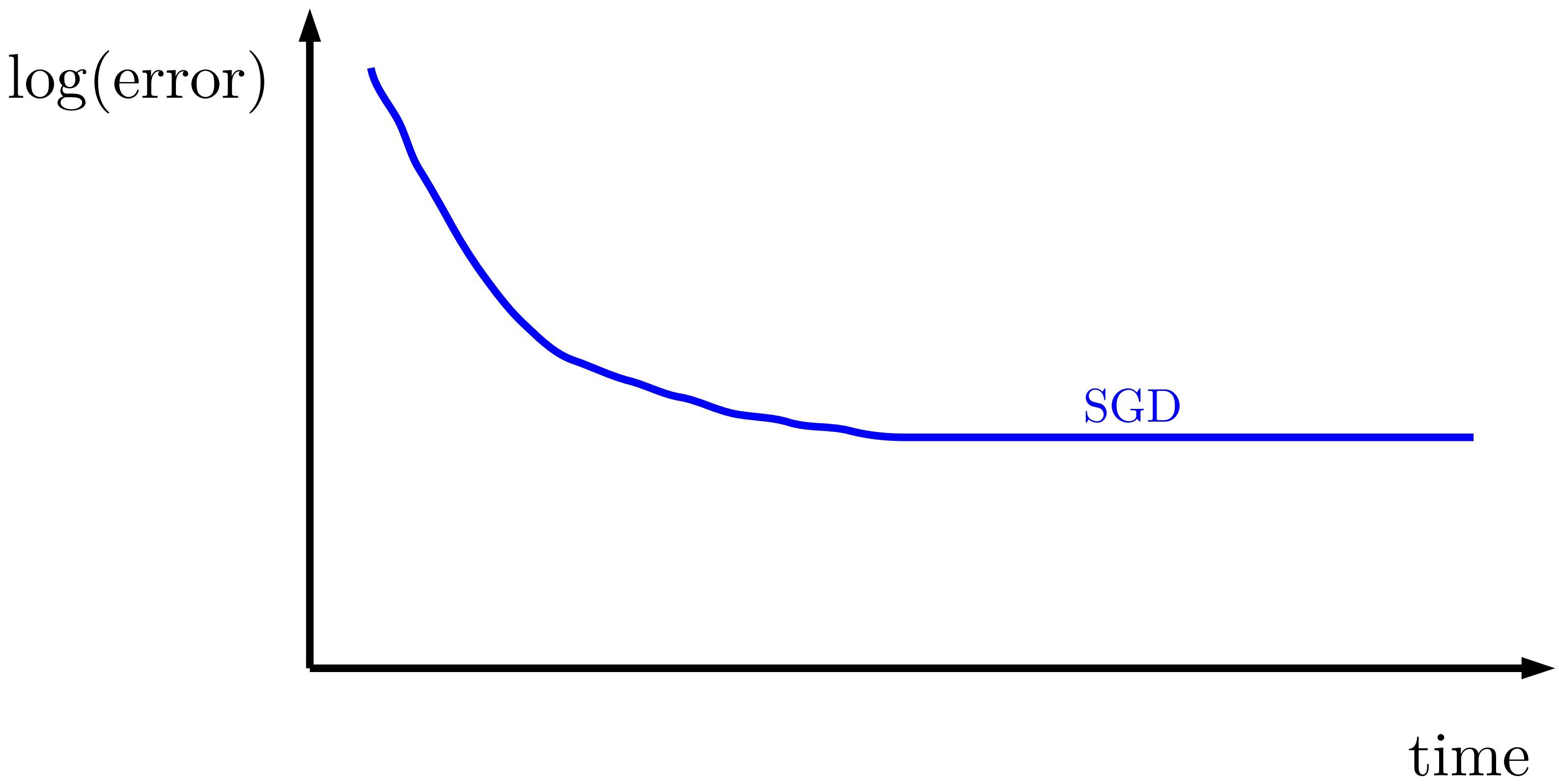
Gradient descent

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

What happens if ϵ is small?

What happens if n is big?

Comparison SGD vs GD



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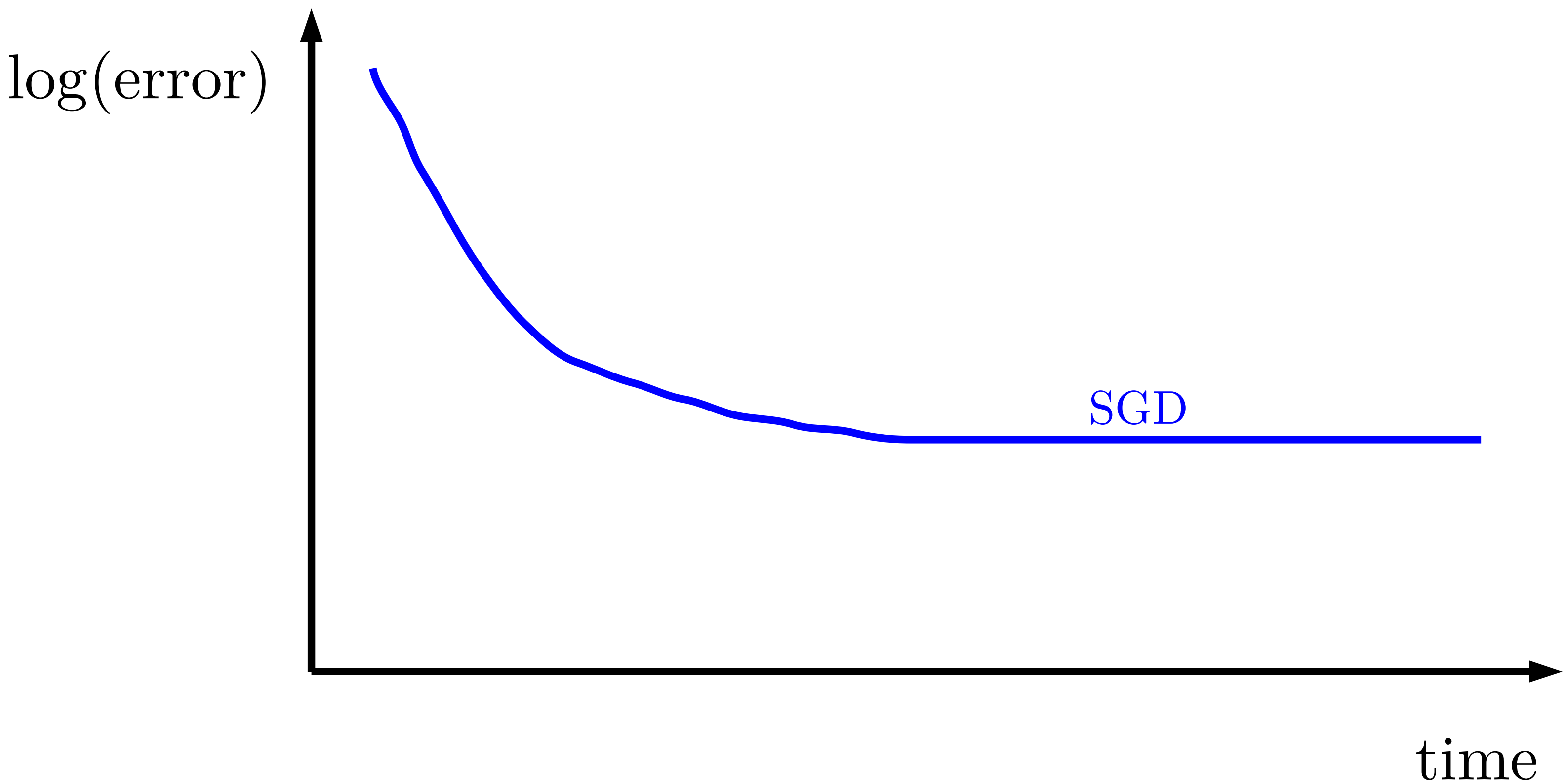
Minimizing Finite Sums with the Stochastic Average Gradient.

Comparison SGD vs GD



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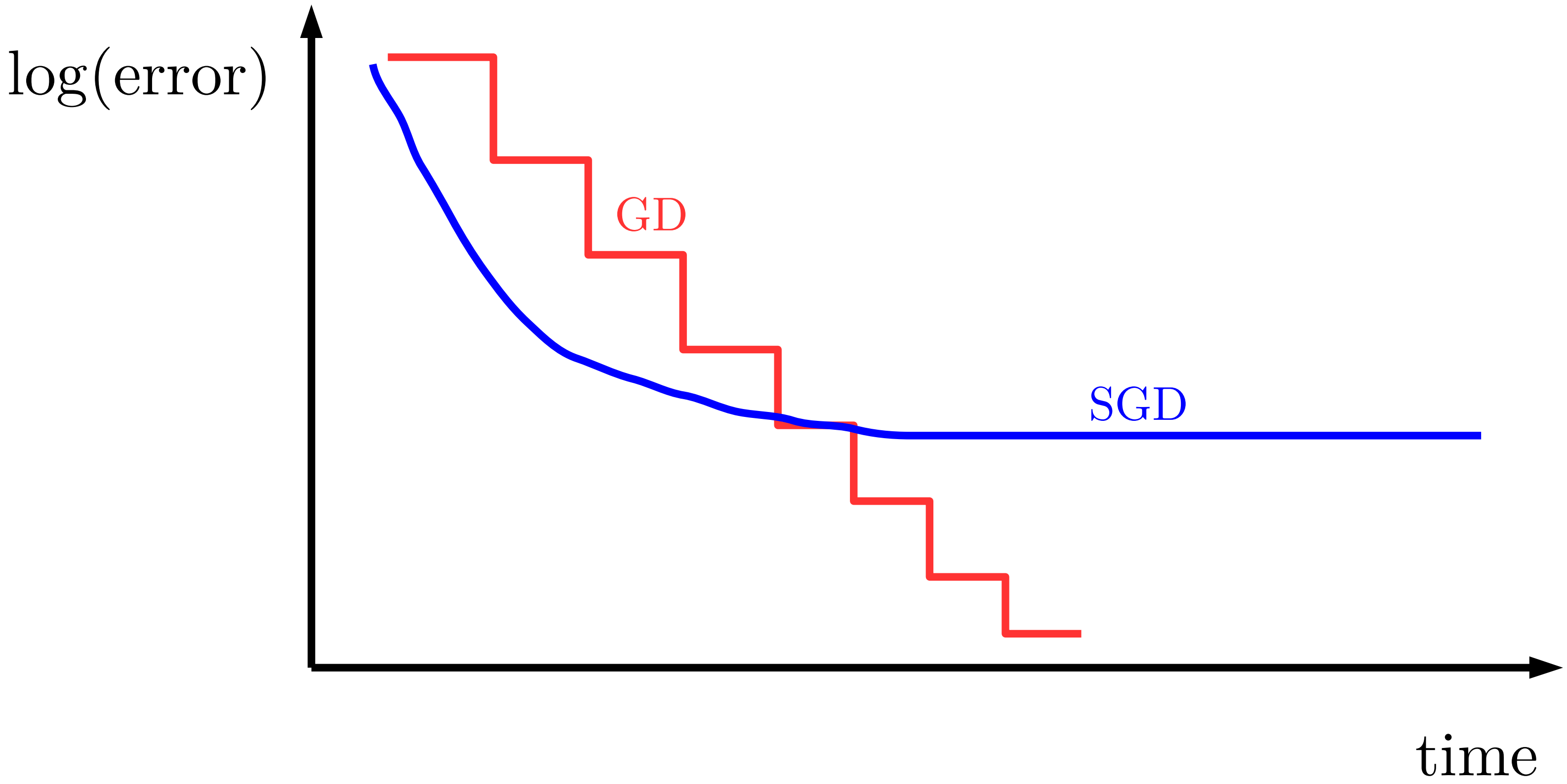

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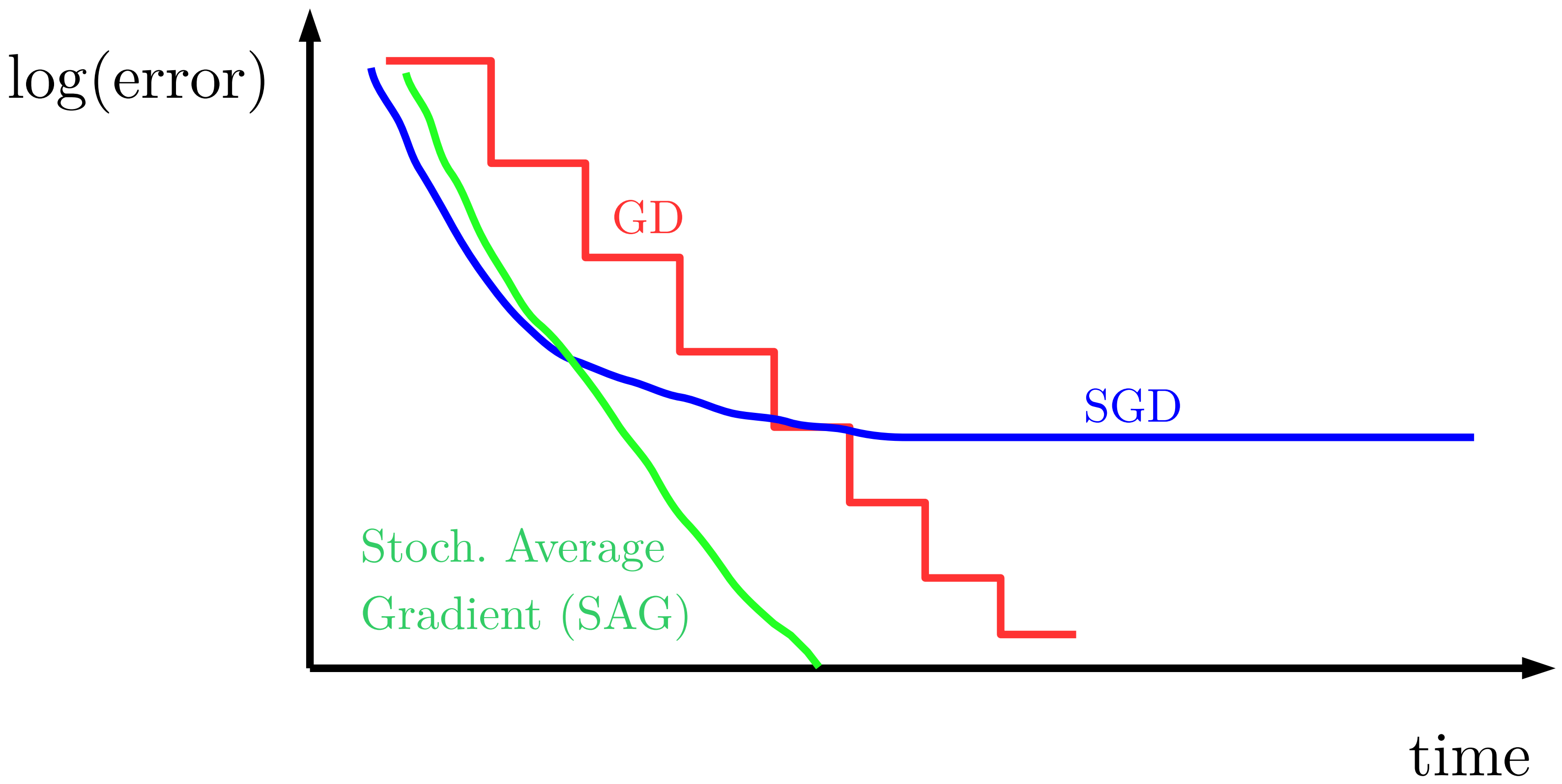

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Why Machine Learners like SGD

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:

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 ∞.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 Convex SGDA

Theorem for SGD 1.1 (Shrinking stepsize)

Let $\overline{w}^T = \dfrac{1}{T}\sum_{t=0}^{T-1} w^t, D = \{x \,:\, ||x|| \leq r\}$ and $r \in \mathbb{R}_+$ such that $||w^*||_2 \leq r$. If $\alpha_t = \dfrac{2r}{B\sqrt{t+1}}$ then

$$\mathbb{E}[f(\overline{w}^T)] - f(w^*) \leq \frac{3rB}{\sqrt{T+1}}$$

SGD 1.1 for Convex

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

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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Sublinear convergence

SGD 1.1 for Convex

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

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 $\overline{w}^T$

Complexity for Convex SGDA

Theorem (Shrinking stepsize)

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

and $\alpha_t = \frac{2}{\lambda(t+1)}$ 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 $\overline{w}^T$

Complexity for Convex SGDA

Theorem (Shrinking stepsize)

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

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

Faster Sublinear convergence

SGD 1.2 for Strongly Convex

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

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

Output $\overline{w}^T$