Revisiting the Polyak Step Size

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Abstract

This note revisits the Polyak step size schedule for convex optimization problems, proving that a simple variant of it simultaneously attains near optimal convergence rates for the gradient descent algorithm, for all ranges of strong convexity, smoothness, and Lipschitz parameters, without a priori knowledge of these parameters.

1 Introduction

Scaleable optimization for machine learning is based entirely on first order gradient methods. Besides the age-old method of stochastic approximation [7], three accelerated methods have proved their practical and theoretical significance: Nesterov acceleration [5], variance reduction [8] and adaptive learning-rate/regularization [4].

Adaptive choices of step sizes allow optimization algorithms to accelerate quickly according to the local curvature and smoothness of the optimization landscape. However, in theory, there are few parameter free algorithms, and, in practice, there are many search heuristics utilized.

Let us examine this question of parameter free, adaptive learning rates for one of the most standard algorithms, namely the gradient descent method:

$$x_{t+1} = x_t - \eta_t \nabla f(x_t).$$

(1)

Although this class of algorithms is not optimal in all settings (i.e. the aforementioned accelerations can be applied), it is fundamental, and we may ask what are optimal known rates along with the optimal step size choices are for this particular algorithm. Here, Table 1 shows the best known rates for gradient descent in the standard regimes: general convex (non-smooth with bounded sub-gradients); β-smooth; α-strongly-convex; and β-smooth&α-strongly convex (see [2],[3] for more details).

| convex       | β-smooth | α-strongly convex | (α, β)-well conditioned |
|--------------|----------|-------------------|-------------------------|
| error        | $\frac{1}{T}$ | $\frac{\beta}{T}$ | $\frac{1}{\alpha T}$ | $e^{-\frac{T}{\alpha \beta}}$ |
| step size    | $\frac{1}{T}$   | $\frac{1}{T}$     | $\frac{1}{\alpha T}$ | $\frac{1}{\beta}$ |

Table 1: Standard convergence rates of gradient descent in convex optimization problems. Error denotes $f(x_t) - f(x^*)$ of a first order methods as a function of the number of iterations. Step Size is the standard learning rate schedule used to obtain this rate. Dependence on other parameters, namely the Lipchitz constant and initial distance to the objective, is omitted.

This work: We show that a single (and simple) choice of a step size schedule gives, simultaneously, the optimal convergence (among the class of gradient descent algorithms) in all these regimes, without knowing these parameters in advance. Perhaps surprisingly, this choice is that prescribed by [6], who argued that this choice was optimal for the non-smooth, convex case (marked as “convex” in Table 1; see also [1]).

2 Convexity Preliminaries

We consider the minimization of a continuous convex function over Euclidean space $f: \mathbb{R}^d \rightarrow \mathbb{R}$ by an iterative gradient-based method. We say that $f$ is α-strongly convex if and only if for all $x, y$:

$$f(y) \geq f(x) + \langle \nabla f(x), y - x \rangle + \frac{\alpha}{2} \|y - x\|^2$$

We say that $f$ is β smooth if and only if for all $x, y$:

$$f(y) \leq f(x) + \langle \nabla f(x), y - x \rangle + \frac{\beta}{2} \|y - x\|^2.$$

The following notation is used throughout:

- $x^* = \arg\min_{x \in \mathbb{R}^d} \{ f(x) \}$ - optimum
• $h(x_t) = h_t = f(x_t) - f(x^*)$ - sub-optimality gap of the iterate
• $d_t = \| x_t - x^* \| -$ Euclidean distance of the iterate.
• $\nabla_t = \nabla f(x_t)$ - gradient of the iterate.
• $\| \nabla_t \|^2$ denotes squared Euclidean norm.

The following are basic properties for $\alpha$-strongly-convex functions and/or $\beta$-smooth functions (proved for completeness in Lemma\[4\]):

$$\frac{\alpha}{2} d_t^2 \leq h_t \leq \frac{\beta}{2} d_t^2, \quad \frac{1}{2\beta} \| \nabla_t \|^2 \leq h_t \leq \frac{1}{2\alpha} \| \nabla_t \|^2 \quad (2)$$

and thus,

$$\frac{1}{4\beta^2} \| \nabla_t \|^2 \leq d_t^2 \leq \frac{1}{4\alpha^2} \| \nabla_t \|^2.$$

The following standard lemma is at the heart of much of the analysis of first order convex optimization.

**Lemma 1.** The sequence of iterates produced by projected gradient descent (equation\[7\]) satisfies:

$$d_{t+1}^2 \leq d_t^2 - 2\eta_t h_t + \eta_t^2 \| \nabla_t \|^2 \quad (3)$$

**Proof.** By algorithm definition we have,

$$d_{t+1}^2 = \| x_{t+1} - x^* \|^2$$
$$= \| x_t - \eta_t \nabla_t - x^* \|^2$$
$$= d_t^2 - 2\eta_t \nabla_t^T (x_t - x^*) + \eta_t^2 \| \nabla_t \|^2$$
$$\leq d_t^2 - 2\eta_t h_t + \eta_t^2 \| \nabla_t \|^2,$$

where we have used properties of convexity in the last step.

\[\square\]

## 3 Main Results

\[6\] argued that, in a sense, the optimal step size choice of $\eta_t$ should decrease the upper bound on $d_{t+1}^2$ as fast as possible. This choice is:

$$\eta_t = \frac{h_t}{\| \nabla_t \|^2}$$

which leads to a decrease of $d_t^2$ by:

$$d_{t+1}^2 \leq d_t^2 - \frac{h_t^2}{\| \nabla_t \|^2}$$

Note that this choice utilizes knowledge of $f(x^*)$, since $h_t = f(x_t) - f(x^*)$.

### Algorithm 1: GD with the Polyak stepsize

1. **Input:** time horizon $T$, $x_0$
2. **for** $t = 0, \ldots, T - 1$ **do**
3. \hspace{1cm} Set $\eta_t = \frac{h_t}{\| \nabla_t \|^2}$
4. \hspace{1cm} $x_{t+1} = x_t - \eta_t \nabla_t$
5. **end for**
6. Return $\hat{x} = x_{\tilde{t}}$ where $\tilde{t} = \arg \min_{t < T} \{ f(x_t) \}$.

\[6\] showed that this choice was optimal for non-smooth convex optimization (i.e. for bounded gradients). Our first result shows that this step size schedule (which knows $f(x^*)$) achieves the min of the best known bounds in all the standard parameter regimes (among the class of projected gradient descent algorithms). Assume $\| \nabla_t \| \leq G$, and define:

$$B_T = \min \left\{ \frac{Gd_0}{\sqrt{T}}, \frac{2\beta d_0^2}{T}, \frac{G^2}{\alpha T}, \frac{\beta d_0^2}{2\beta} \left( 1 - \frac{\alpha}{2\beta} \right)^T \right\}.$$

**Theorem 1.** (GD with the Polyak Step Size) Algorithm\[7\] attains the following regret bound after $T$ steps:

$$f(\hat{x}) - f(x^*) \leq B_T$$

Without knowledge of the optimal function value $f(x^*)$, our second main result shows that all we need is a lower bound $\hat{f}_0 \leq f(x^*)$, and we can do nearly as well as the exact Polyak step size method (up to a log factor in $f(x^*) - \hat{f}_0$). Note that it is often the case that $\hat{f}_0 = 0$ is a valid lower bound (e.g. in empirical risk minimization settings).

**Theorem 2.** (The Adaptive Polyak Step Size) Assume a lower bound $\hat{f}_0 \leq f(x^*)$: that $K = 1 + \left\lceil 2 \log \left( \frac{f(x^*) - \hat{f}_0}{B_T} \right) \right\rceil$. Algorithm\[5\] returns an $\hat{x}$ such that:

$$f(\hat{x}) - f(x^*) \leq 2B_T$$

Furthermore, the number of gradient descent updates made by the algorithm is at most $T \cdot (1 + \left\lceil 2 \log \left( \frac{f(x^*) - \hat{f}_0}{B_T} \right) \right\rceil)$.

In other words, this algorithm makes at most $O(T \cdot \log \left( \frac{f(x^*) - \hat{f}_0}{B_T} \right))$ gradient updates to get $B_T$ error, while the exact Polyak stepsize uses $T$ updates (to obtain $B_T$ error). The subtlety in the construction is that even with a initial lower bound on $\hat{f}_0$, the values $f(x_t)$ are only upper bounds. However, Algorithm\[5\] and its proof shows how either the lower bound can be refined or, if not, the algorithm will succeed. Note that Algorithm\[5\] always call the subroutine Algorithm\[2\] starting at the same $x_0$.  

Algorithm 2 GD with a lower bound

1: Input: time horizon $T$, $x_0$, lower bound $\tilde{f} \leq f(x^*)$.
2: for $t = 0, \ldots, T - 1$ do
3: \quad Set $\eta_t = \frac{f(x_t) - \tilde{f}}{\|\nabla f(x_t)\|^2}$
4: \quad $x_{t+1} = x_t - \eta_t \nabla f(x_t)$
5: end for
6: Return $\bar{x} = x_t$, where $t^* = \text{argmin}_{t < T} \{f(x_t)\}$.

Algorithm 3 Adaptive Polyak

1: Input: time horizon $T$, number of epochs $K$, $x_0$, value $\tilde{f}_0 \leq f(x^*)$.
2: for epoch $k = 0, \ldots, K - 1$ do
3: \quad Let $\bar{x}_k$ be the output of Algorithm 2 using input $x_0, T, \bar{f}_k$.
4: \quad Update $\bar{f}_{k+1} \leftarrow \frac{f(\bar{x}_k) + \tilde{f}_k}{2}$
5: end for
6: Return $\bar{x}_k$, where $k^* = \text{argmin}_{k < K} \{f(\bar{x}_k)\}$.

3.1 Analysis: the exact case

Theorem 1 directly follows from the following lemma. It is helpful for us to state this lemma in a more general form, where, for $0 \leq \gamma \leq 1$, we define $R_{T, \gamma}$ as follows:

$$R_{T, \gamma} = \min \left\{ \frac{Gd_0}{\sqrt{T}} \cdot \frac{2\beta d_0^2}{\gamma T}, \frac{G^2}{\gamma \alpha T}, \beta d_0^2 \left( 1 - \frac{\alpha}{\beta} \right)^T \right\}.$$  \(^1\)

Lemma 2. For $0 \leq \gamma \leq 1$, suppose that a sequence $x_0, \ldots, x_t$ satisfies:

$$d_{t+1}^2 \leq d_t^2 - \gamma \frac{h_t^2}{\|\nabla f_t\|^2}$$  \(^2\)

then for $\bar{x} = x_{t^*}$, where $t^* = \text{argmin}_{t < T} \{f(x_t)\}$,

$$h(\bar{x}) \leq R_{T, \gamma}.$$  \(^3\)

Proof. The proof analyzes different cases:

1. For convex functions with gradient bound $G$,

$$d_{t+1}^2 - d_t^2 \leq -\frac{\gamma h_t^2}{\|\nabla f_t\|^2} \leq -\frac{\gamma h_t^2}{G^2}.$$  

Summing up over $T$ iterations, and using Cauchy-Schwartz, we have

$$\frac{1}{T} \sum_t h_t \leq \frac{1}{\sqrt{T}} \sqrt{\sum_t h_t^2} \leq \frac{Gd_0}{\sqrt{T}} \sqrt{\sum_t (d_t^2 - d_{t+1}^2)} \leq \frac{Gd_0}{\sqrt{T}}.$$  

2. For smooth functions, equation \(^2\) implies:

$$d_{t+1}^2 - d_t^2 \leq -\gamma h_t^2 \leq -\gamma \frac{h_t^2}{2\beta}. $$  

This implies

$$\frac{1}{T} \sum_t h_t \leq \frac{2\beta d_0^2}{\gamma T}. $$  

3. For strongly convex functions, equation \(^2\) implies:

$$d_{t+1}^2 - d_t^2 \leq -\gamma \frac{h_t^2}{\|\nabla f_t\|^2} \leq -\gamma \frac{h_t^2}{G^2} \leq -\gamma \frac{\alpha^2 d_t^2}{4G^2}. $$  

In other words, $d_{t+1}^2 \leq d_t^2 (1 - \gamma \frac{\alpha^2 d_t^2}{4G^2})$. Defining $a_t := \gamma \frac{\alpha^2 d_t^2}{4G^2}$, we have:

$$a_{t+1} \leq a_t (1 - a_t). $$

This implies that $a_t \leq \frac{1}{T}$, which can be seen by induction. The proof is completed as follows:\(^4\):

$$\frac{1}{T^2} \sum_{t=T/2}^T h_t^2 \leq \frac{2G^2}{\gamma T} \sum_{t=T/2}^T (d_t^2 - d_{t+1}^2) \leq \frac{2G^2}{\gamma^2} (d_{T/2}^2 - d_T^2) \leq \frac{G^4}{\gamma^2 \alpha^2 T^2}.$$  

Thus, there exists a $t$ for which $h_t^2 \leq \frac{G^4}{\gamma^2 \alpha^2 T^2}$. Taking the square root completes the claim.

4. For both strongly convex and smooth:

$$d_{t+1}^2 - d_t^2 \leq -\gamma \frac{h_t^2}{\|\nabla f_t\|^2} \leq -\gamma \frac{h_t^2}{2\beta} \leq -\gamma \frac{\alpha d_t^2}{\beta}. $$  

Thus,

$$h_t \leq \beta d_t^2 \leq \beta d_0^2 \left( 1 - \frac{\alpha}{\beta} \right)^T.$$  

This completes the proof of all cases.  \(\square\)

\(^1\)That $a_0 \leq 1$ follows from equation \(^2\). For $t = 1$, $a_1 \leq \frac{1}{2}$ since $a_1 \leq a_0 (1 - a_0)$ and $0 \leq a_0 \leq 1$. For the induction step, $a_t \leq a_{t-1} (1 - a_{t-1}) \leq \frac{1}{2} (1 - 1) = \frac{1}{2}$, which follows from $\frac{1}{T}$.

\(^2\)This assumes $T$ is even. $T$ odd leads to the same constants.
3.2 Analysis: the adaptive case

The proof of Theorem 2 rests on the following lemma which shows that, given a lower bound on the objective, the subroutine in Algorithm 2 either returns a near-optimal point with desired precision or a tighter lower bound.

Lemma 3. Assume $\|\nabla f\| \leq G$. With input $T$, $x_0$, and $\tilde{f}$ where $\tilde{f} \leq f(x^*)$, Algorithm 2 returns a point $\tilde{x}$ such that one of the following holds:

1. $h(\tilde{x}) \leq R_T, 2$
2. For $\tilde{f}_+ := \frac{f(x_0) + \tilde{f}}{2}$,

$$0 \leq f(x^*) - \tilde{f}_+ \leq \frac{f(x^*) - \tilde{f}}{2}$$

Proof. Due to that $\tilde{f}$ is a lower bound, we have that

$$\eta_t = \frac{f(x_t) - \tilde{f}}{2\|\nabla l\|^2} \geq \frac{h_t}{2\|\nabla l\|^2}.$$  

We will consider two cases. First, suppose that

$$\eta_t \leq \frac{h_t}{\|\nabla l\|^2}$$

held for $T$ steps. For this case, by Lemma 1

$$d_{t+1}^2 \leq d_t^2 - 2\eta_t h_t + \eta_t^2 \|\nabla l\|^2$$

$$= d_t^2 - \eta_t h_t$$

$$\leq d_t^2 - \frac{h_t^2}{2\|\nabla l\|^2}$$

using the assumed upper bound on $\eta_t$ in the second step and the lower bound in the last step. By Lemma 2 we can take $\gamma = 1/2$ and we have that $\min_{1 \leq T \leq \tilde{T}} h_t \leq R_T, 2$.

Now suppose there exists a time $t^*$ where Equation 5 fails to hold. Hence, for some iteration,

$$\eta_{t^*} = \frac{f(x_{t^*}) - \tilde{f}}{2\|\nabla l\|^2} \geq \frac{f(x_{t^*}) - f(x^*)}{\|\nabla l\|^2}.$$  

After rearranging, we have

$$f(x^*) \geq \frac{f(x_{t^*}) + \tilde{f}}{2} \geq \frac{f(x) + \tilde{f}}{2} = \tilde{f}_+.$$  

using the definition of $x$ and the definition of $\tilde{f}_+$. Hence, $f(x^*) - \tilde{f}_+ \geq 0$. In addition, we have

$$f(x^*) - \tilde{f}_+ = f(x^*) - \frac{f(x) + \tilde{f}}{2}$$

$$\leq f(x^*) - \frac{f(x^*) + \tilde{f}}{2}$$

$$= f(x^*) - \tilde{f}$$

which completes the proof.

Now the proof Theorem 2 follows.

Proof. (of Theorem 2) Note $R_T, \tilde{T} \leq 2B_T$. Suppose that $f(x_k) - f(x^*) \geq R_T, \tilde{T}$ for all $k \leq K - 1$, else the proof would be complete. By Lemma 3 we have that $f(x^*) - \tilde{f}_k \leq (1/2)^k (f(x^*) - \tilde{f}_0)$ and that $0 \leq f(x^*) - \tilde{f}_k$, for all $k \in \{1, \ldots, K\}$. Hence, for $k = K - 1 = [2 \log \frac{f(x^*) - \tilde{f}_0}{B_T}]$, we have $f(x^*) - \tilde{f}_{K-1} \leq B_T$. By construction $\tilde{f}_K = \frac{f(x_{K-1}) + \tilde{f}_{K-1}}{2}$, which implies:

$$f(\tilde{x}_{K-1}) = 2\tilde{f}_K - \tilde{f}_{K-1}$$

$$\leq 2f(x^*) - \tilde{f}_{K-1}$$

$$= f(x^*) + f(x^*) - \tilde{f}_{K-1}$$

$$\leq f(x^*) + B_T,$$

which completes the proof.

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## A Elementary properties of convex analysis

**Lemma 4.** The following properties hold for α-strongly-convex functions and/or β-smooth functions.

1. \( \frac{\alpha}{2} d_t^2 \leq h_t \)
2. \( h_t \leq \frac{\alpha}{2} d_t^2 \)
3. \( \frac{1}{\alpha} \| \nabla \ell \|_2^2 \leq h_t \)
4. \( h_t \leq \frac{1}{\alpha} \| \nabla \ell \|_2^2 \)

**Proof.**

**Claim 1:** \( h_t \geq \frac{\alpha}{2} d_t^2 \)

By strong convexity, we have

\[
h_t = f(x_t) - f(x^*) \geq \nabla f_t(x^*)(x_t - x^*) + \frac{\alpha}{2} \|x_t - x^*\|^2
\]

where the last inequality holds by optimality conditions for \( x^* \).

**Claim 2:** \( h_t \leq \beta d_t^2 \)

By smoothness,

\[
h_t = f(x_t) - f(x^*) \leq \nabla f_t(x^*)(x_t - x^*) + \frac{\beta}{2} \|x_t - x^*\|^2
\]

where the last inequality follows since the gradient at the global optimum is zero.

**Claim 3:** \( h_t \geq \frac{1}{\beta} \| \nabla \ell \|_2^2 \)

Using smoothness:

\[
h_t = f(x_t) - f(x^*) \geq \{ f(x_t) - f(x_{t+1}) \}
\]

\[
\geq \{ \nabla f_t(x_t)(x_{t+1} - x_t) - \frac{\beta}{2} \|x_t - x_{t+1}\|^2 \}
\]

\[
= \eta \| \nabla \ell \|_2^2 - \frac{\beta}{2} \eta^2 \| \nabla \ell \|_2^2
\]

\[
\geq \frac{1}{2\beta} \| \nabla \ell \|_2^2.
\]

**Claim 4:** \( h_t \leq \frac{1}{\alpha} \| \nabla \ell \|_2^2 \)

We have for any pair \( x, y \in \mathbb{R}^d \):

\[
 f(y) \geq f(x) + \nabla f(x)^T (y - x) + \frac{\alpha}{2} \|x - y\|^2
\]

\[
\geq \min_{z \in \mathbb{R}^d} \{ f(x) + \nabla f(x)^T (z - x) + \frac{\alpha}{2} \|x - z\|^2 \}
\]

\[
= f(x) - \frac{1}{2\alpha} \| \nabla f(x) \|^2.
\]

by \( z = x - \frac{1}{\alpha} \nabla f(x) \)

In particular, taking \( x = x_t, y = x^* \), we have

\[
h_t = f(x_t) - f(x^*) \leq \frac{1}{2\alpha} \| \nabla \ell \|_2^2.
\]

This completes the proof. \( \square \)