Revisiting the Polyak step size

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Abstract

This paper 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-priory 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:

$$\mathbf{x}_{t+1} = \mathbf{x}_t - \eta_t \nabla f(\mathbf{x}_t) \,. \tag{1}$$

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).

From a practical perspective these step size settings are unfortunately disparate in various regimes: ranging

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

Table 1: Standard convergence rates of gradient descent in convex optimization problems. Error denotes $f(\mathbf{x}_t) - f(\mathbf{x}^*)$ 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.

from rapidly decaying at $\eta_t = O(\frac{1}{\alpha t})$ to moderately decaying at $\eta_t = O(\frac{1}{\sqrt{t}})$ to a constant $\eta_t = \frac{1}{\beta}$ (see [2, 3] for more details).

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]).

An important future direction is, if we enrich the class of update rules (say to included momentum based methods or stochastic update rules) then can we also obtain optimal algorithms with no knowledge of the underlying curvature of the problem.

2 Convexity Preliminaries

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

$$f(\mathbf{y}) \ge f(\mathbf{x}) + \nabla f(\mathbf{x})(\mathbf{y} - \mathbf{x}) + \frac{\alpha}{2} \|\mathbf{x} - \mathbf{y}\|^2$$

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We say that f is β smooth if and only if $\forall \mathbf{x}, \mathbf{y}$:

$$f(\mathbf{y}) \le f(\mathbf{x}) + \nabla f(\mathbf{x})(\mathbf{y} - \mathbf{x}) + \frac{\beta}{2} \|\mathbf{x} - \mathbf{y}\|^2$$

The following notation is used throughout:

- $\mathbf{x}^{\star} = \operatorname{argmin}_{\mathbf{x} \in \mathbb{R}^d} \{f(\mathbf{x})\}$ optimum
- $h(\mathbf{x}_t) = h_t = f(\mathbf{x}_t) f(\mathbf{x}^{\star})$ distance to optimality
- $d_t = \|\mathbf{x}_t \mathbf{x}^{\star}\|$ Euclidean distance of the iterate.
- $\nabla_t = \nabla f(\mathbf{x}_t)$ gradient of the iterate.
- $\|\nabla_t\|^2$ denotes squared Euclidean norm.

The following are basic properties for α -strongly-convex $h_t = f(\mathbf{x}_t) - f(\mathbf{x}^*)$. functions and/or β -smooth functions (proved for completence) [6] showed that the convex optimization (6) showed that the convex optimization (7) of β and β and β are the function of β and β and β are the function of β are the function of β are the function of β and β are the function of β and β are the function of β and β are the function of β are the function of β and β are the function of β and β are the function of β a

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

and thus,

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

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 1) satisfies:

$$d_{t+1}^2 \le d_t^2 - 2\eta_t h_t + \eta_t^2 \|\nabla_t\|^2 \tag{3}$$

Proof. By algorithm definition we have,

$$d_{t+1}^2 = \|\mathbf{x}_{t+1} - \mathbf{x}^\star\|^2$$

= $\|\mathbf{x}_t - \eta_t \nabla_t - \mathbf{x}^\star\|^2$
= $d_t^2 - 2\eta_t \nabla_t^\top (\mathbf{x}_t - \mathbf{x}^\star) + \eta_t^2 \|\nabla_t\|^2$
 $\leq d_t^2 - 2\eta_t h_t + \eta_t^2 \|\nabla_t\|^2$

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

3 Main Results

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

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

1: Input: time horizon T, x_0 2: for t = 0, ..., T - 1 do 3: Set $\eta_t = \frac{h_t}{\|\nabla_t\|^2}$ 4: $\mathbf{x}_{t+1} = \mathbf{x}_t - \eta_t \nabla_t$ 5: end for 6: Return $\bar{\mathbf{x}} = \operatorname{argmin}_{\mathbf{x}_t} \{f(\mathbf{x}_t)\}$

which leads to a decrease of d_t^2 by:

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

Note that this choice utilizes knowledge of $f(\mathbf{x}^*)$, since $h_t = f(\mathbf{x}_t) - f(\mathbf{x}^*)$.

[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 $f(\mathbf{x}^*)$) 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:

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

Theorem 1. (GD with the Polyak Step Size) Algorithm 1 attains the following regret bound after T steps:

$$h(\bar{\mathbf{x}}) = \min_{0 \le t \le T} \{h_t\} \le B_T$$

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

Theorem 2. (*The Adaptive Polyak Step Size*) Assume a lower bound $\tilde{f}_0 \leq f(\mathbf{x}^*)$; that $K = \log \frac{f(\mathbf{x}^*) - \tilde{f}_0}{B_T}$. Algorithm 3 returns an $\bar{\mathbf{x}}$ such that:

$$f(\bar{\mathbf{x}}) - f(\mathbf{x}^{\star}) \le 2B_T$$

Furthermore, the algorithm makes at most $T \cdot \log \frac{f(\mathbf{x}^*) - f_0}{B_T}$ gradient descent updates.

In other words, this algorithms makes at most $T \cdot \log \frac{f(\mathbf{x}^*) - f_0}{B_T}$ 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

Algorithm 2 GD with a lower bound

1: Input: time horizon T, x_0 , lower bound $\tilde{f} \leq f(\mathbf{x}^*)$. 2: for t = 0, ..., T - 1 do 3: Set $\eta_t = \frac{f(\mathbf{x}_t) - \tilde{f}}{2 \|\nabla_t\|^2}$ 4: $\mathbf{x}_{t+1} = \mathbf{x}_t - \eta_t \nabla_t$ 5: end for 6: Return $\bar{\mathbf{x}} = \operatorname{argmin}_{\mathbf{x}_t} \{f(\mathbf{x}_t)\}$

Algorithm 3 Adaptive Polyak

- Input: time horizon *T*, number of epochs *K*, *x*₀, value *f*₀ ≤ *f*(**x***).
 for epoch *k* = 0, ..., *K* − 1 do
 Run Algorithm 2 with *x*₀, *T*, *f*_k to obtain *x*̄.
 Update *f*_{k+1} ← *f*(*x*) − *f*_k/2
 end for
- 6: Return $\bar{\mathbf{x}}$
- 6: Return

bound on \tilde{f}_0 , the values $f(\mathbf{x}_t)$ are only upper bounds. However, Algorithm 3 and its proof shows how either the lower bound can be refined or, if not, the algorithm will succeed. Note that Algorithm 3 always call the subroutine Algorithm 2 starting at the same x_0 .

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 $0 \le \gamma \le 1$, we define $R_{T,\gamma}$ as follows:

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

Lemma 2. For $0 \le \gamma \le 1$, suppose that a sequence $\mathbf{x}_0, \ldots \mathbf{x}_t$ satisfies:

$$d_{t+1}^2 \le d_t^2 - \gamma \frac{h_t^2}{\|\nabla_t\|^2} \tag{4}$$

then for $\bar{\mathbf{x}}$ as defined in the algorithm, we have:

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

Proof. The proof analyzes different cases:

1. For convex functions with gradient bound G,

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

Summing up over T iterations, and using Cauchy-

Schwartz, we have

$$\frac{1}{T} \sum_{t} h_{t} \leq \frac{1}{\sqrt{T}} \sqrt{\sum_{t} h_{t}^{2}}$$
$$\leq \frac{G}{\sqrt{\gamma T}} \sqrt{\sum_{t} (d_{t}^{2} - d_{t+1}^{2})} \leq \frac{Gd_{0}}{\sqrt{\gamma T}}$$

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

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

This implies

$$\frac{1}{T} \sum_{t} h_t \le \frac{2\beta d_0^2}{\gamma T} \,.$$

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

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

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

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

This implies that $a_t \leq \frac{1}{t+1}$, which can be seen by induction¹. The proof is completed as follows²:

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

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:

$$d_{t+1}^2 - d_t^2 \le -\gamma \frac{h_t^2}{\|\nabla_t\|^2} \le -\frac{\gamma h_t}{2\beta} \le -\gamma \frac{\alpha}{\beta} d_t^2$$

Thus,

$$\underline{h_T \leq \beta d_T^2 \leq \beta d_0^2 \left(1 - \gamma \frac{\alpha}{\beta}\right)^T}.$$

¹That $a_0 \leq 1$ 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, $a_t \leq a_{t-1}(1-a_{t-1}) \leq \frac{1}{t}(1-\frac{1}{t}) = \frac{t-1}{t^2} = \frac{1}{t+1}(\frac{t^2-1}{t^2}) \leq \frac{1}{t+1}$. ²This assumes T is even. T odd leads to the same constants This completes the proof of all cases.

3.2 Analysis: the adaptive case

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

Lemma 3. Assume $\|\nabla_t\| \leq G$ and that $\tilde{f} \leq f(\mathbf{x}^*)$. Algorithm 2 returns a point $\bar{\mathbf{x}}$ such that one of the following holds:

1. $h(\bar{\mathbf{x}}) \leq R_{T,\frac{1}{2}}$ 2. For $\tilde{f}_+ := \frac{f(\bar{\mathbf{x}}) - \tilde{f}}{2}$, $0 \leq f(\mathbf{x}^{\star}) - \tilde{f}_+ \leq \frac{f(\mathbf{x}^{\star}) - \tilde{f}}{2}$

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

$$\eta_t = \frac{f(\mathbf{x}_t) - \hat{f}}{2||\nabla_t||^2} \ge \frac{h_t}{2||\nabla_t||^2}$$

We will consider two cases. First, suppose that

$$\eta_t \le \frac{h_t}{\|\nabla_t\|^2} \tag{5}$$

held for T steps. For this case, by lemma 1,

$$\begin{array}{rcl} d_{t+1}^2 &\leq& d_t^2 - 2\eta_t h_t + \eta_t^2 \|\nabla_t\|^2 \\ &\leq& d_t^2 - 2\eta_t h_t + \eta_t h_t \\ &=& d_t^2 - \eta_t h_t \\ &\leq& d_t^2 - \frac{h_t^2}{2||\nabla_t||^2} \end{array}$$

using the assumed upper bound on η_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 $\min_{t < T} h_t \leq R_{T,\frac{1}{2}}$.

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

$$\eta_{t^*} = \frac{f(\mathbf{x}_{t^*}) - \tilde{f}}{2||\nabla_{t^*}||^2} \ge \frac{f(\mathbf{x}_{t^*}) - f(\mathbf{x}^*)}{||\nabla_{t^*}||^2}$$

After rearranging, we have

$$f(\mathbf{x}^{\star}) \geq \frac{f(\mathbf{x}_{t^{\star}}) + \tilde{f}}{2} \geq \frac{f(\bar{\mathbf{x}}) - \tilde{f}}{2} = \tilde{f}_{+}.$$

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

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

$$\leq f(\mathbf{x}^{\star}) - \frac{f(x^{\star}) - \tilde{f}}{2}$$

$$= \frac{f(\mathbf{x}^{\star}) - \tilde{f}}{2}$$

which completes the proof.

Now the proof Theorem 2 follows.

Proof. (of Theorem 2) Note that $R_{T,\frac{1}{2}} = B_T$. To see that Theorem 2 follows we can suppose that condition 1 above does not occur in $\log \frac{f(\mathbf{x}^*) - \tilde{f}_0}{B_T}$ calls to the subroutine, algorithm 2. This implies that at the last call $f(\mathbf{x}^*) - \tilde{f} \leq B_T$ (since this lower bound halves for each subroutine call). Now since $0 \leq f(\mathbf{x}^*) - \tilde{f}_+$ we have that by definition of \tilde{f}_+ that $f(\bar{\mathbf{x}}) \leq 2f(\mathbf{x}^*) - \tilde{f} = f(\mathbf{x}^*) + f(\mathbf{x}^*) - \tilde{f} \leq f(\mathbf{x}^*) + B_T$.

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A Elementary properties of convex analysis

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

1. $\frac{\alpha}{2}d_t^2 \leq h_t$

2.
$$h_t \leq \frac{\beta}{2} d_t^2$$

3. $\frac{1}{2\beta} \|\nabla_t\|^2 \le h_t$

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

Proof. 1. case 1: $h_t \ge \frac{\alpha}{2} d_t^2$

By strong convexity, we have

$$h_t = f(\mathbf{x}_t) - f(\mathbf{x}^*)$$

$$\geq \nabla f_t(\mathbf{x}^*)(\mathbf{x}_t - \mathbf{x}^*) + \frac{\alpha}{2} \|\mathbf{x}_t - \mathbf{x}^*\|^2$$

$$\geq \frac{\alpha}{2} \|\mathbf{x}_t - \mathbf{x}^*\|^2$$

where the last inequality holds by optimality conditions for \mathbf{x}^* .

2. case 2: $h_t \leq \beta d_t^2$

By smoothness,

$$h_t = f(\mathbf{x}_t) - f(\mathbf{x}^*)$$

$$\leq \nabla f_t(\mathbf{x}^*)(\mathbf{x}_t - \mathbf{x}^*) + \frac{\beta}{2} \|\mathbf{x}_t - \mathbf{x}^*\|^2$$

$$\leq \frac{\beta}{2} \|\mathbf{x}_t - \mathbf{x}^*\|^2$$

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

3. case 3: $h_t \geq \frac{1}{\beta} \|\nabla_t\|^2$ Using smoothness:

$$h_t = f(\mathbf{x}_t) - f(\mathbf{x}^*)$$

$$\geq \{f(\mathbf{x}_t) - f(\mathbf{x}_{t+1})\}$$

$$\geq \left\{\nabla f_t(\mathbf{x}_t)(\mathbf{x}_{t+1} - \mathbf{x}_t) - \frac{\beta}{2} \|\mathbf{x}_t - \mathbf{x}_{t+1}\|^2\right\}$$

$$= \eta \|\nabla_t\|^2 - \frac{\beta}{2}\eta^2 \|\nabla_t\|^2$$

$$\geq \frac{1}{2\beta} \|\nabla_t\|^2,$$

4. case 3: $h_t \leq \frac{1}{\alpha} \|\nabla_t\|^2$ We have for any pair $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$:

$$\begin{split} f(\mathbf{y}) &\geq f(\mathbf{x}) + \nabla f(\mathbf{x})^{\top} (\mathbf{y} - \mathbf{x}) + \frac{\alpha}{2} \|\mathbf{x} - \mathbf{y}\|^2 \\ &\geq \min_{\mathbf{z} \in \mathbb{R}^d} \left\{ f(\mathbf{x}) + \nabla f(\mathbf{x})^{\top} (\mathbf{z} - \mathbf{x}) + \frac{\alpha}{2} \|\mathbf{x} - \mathbf{z}\|^2 \right\} \\ &= f(\mathbf{x}) - \frac{1}{2\alpha} \|\nabla f(\mathbf{x})\|^2. \\ &\text{by } \mathbf{z} = \mathbf{x} - \frac{1}{\alpha} \nabla f(\mathbf{x}) \end{split}$$

In particular, taking $\mathbf{x} = \mathbf{x}_t$, $\mathbf{y} = \mathbf{x}^*$, we get

$$h_t = f(\mathbf{x}_t) - f(\mathbf{x}^*) \le \frac{1}{2\alpha} \|\nabla_t\|^2.$$
 (6)