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Divergence of the ADAM algorithm with fixed-stepsize: a (very) simple example

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Abstract

A very simple unidimensional function with Lipschitz continuous gradient is constructed such that the ADAM algorithm with constant stepsize, started from the origin, diverges when applied to minimize this function in the absence of noise on the gradient. Divergence occurs irrespective of the choice of the method parameters.

Keywords: ADAM algorithm, machine learning, deterministic nonconvex optimization.

1 Introduction

This short note provides a new explicit example of failure of the ADAM algorithm [3], one of the most popular training methods in machine learning. Given the problem

$$\min_{x \in \mathbb{R}^n} f(x) \tag{1}$$

where f is continuously differentiable function from \mathbb{R}^n into \mathbb{R} with Lipschitz continuous gradient, and a starting iterate x_0 , the ADAM sequence of iterates is defined (see [4]), for $i \in \{1, \dots, n\}$ and $k \geq 0$, by the recurrences

$$[m_k]_i = \beta_1 [m_{k-1}]_i + (1 - \beta_1) [g_k]_i, \tag{2}$$

$$[v_k]_i = \beta_2 [v_{k-1}]_i + (1 - \beta_2) [g_k]_i^2, \tag{3}$$

$$[x_{k+1}]_i = [x_k]_i - \alpha \frac{[m_k]_i}{\sqrt{[v_k]_i}}, \tag{4}$$

where $[v]_i$ is the i -th component of the vector $v \in \mathbb{R}^n$, m_k is the k -th “momentum”, x_k is the k -th iterate, $g_k = \nabla_x^1 f(x_k)$, $\beta_1 \in [0, 1)$ is the momentum parameter and $\beta_2 \in [0, 1)$ is the “forgetting” parameter, and $\alpha > 0$ is a (fixed) steplength/learning-rate parameter. The recurrences (2) and (3) are initialized by setting, for $i \in \{1, \dots, n\}$, $[m_{-1}]_i = [g_0]_i$ and $[v_{-1}]_i = [g_0]_i^2$, respectively. ADAM is intended to converge to find first-order points for problem (1), in the sense that, for each $i \in \{1, \dots, n\}$, $|[g_k]_i|$ should converge to zero when k tends to infinity. In practice, this algorithm is most often used in a stochastic context where the gradient g_k is contaminated by noise (typically resulting from sampling) and has generated a considerable interest in the machine learning community.

Despite its widespread use, difficulties with this algorithm are not new. In the noiseless (deterministic/full batch) case, obstacles for proving convergence were in particular mentioned in [2], essentially pointing out the possibility that second-order terms in the Taylor’s expansion of the objective function could not vanish quickly enough. In [4, Theorem 1] an example of non

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convergence on a convex function was produced in the online-learning stochastic context, but this example crucially depends on the nonzero variance of the noise. In a recent discussion at the June 2023 Thematic Einstein Semester on Optimization and Machine Learning in Berlin, it was suggested that, although likely, no explicit example of failure of Adam with fixed stepsize was available for the deterministic case (where the variance is zero). This prompted the author to produce the (very simple) one which is, for the record, detailed in the next section. We note that an again convex but deterministic example had already been provided in the comprehensive analysis of ADAM's behaviour (with decreasing stepsize) detailed in [5] (see Propositions 3.3 and E1). This analysis describes conditions which delineate a region strictly included in $[0, 1]^2$ such that ADAM with parameters β_1 and β_2 chosen in this region generates a diverging sequence on this example. In contrast, the simple example we are about to discuss is nonconvex and applies to the entire $[0, 1]^2$, but requires constant stepsize. It can therefore be seen as complementing the analysis of [5].

2 The example

To show that the ADAM algorithm may fail to converge on nonconvex functions with Lipschitz gradient, we will exhibit an example in dimension one, which we construct in two stages. We first define sequences of iterates, together with associated function and gradient values which remain constant throughout the iterations. We next verify that these sequences may be considered as generated by applying the ADAM algorithm to a nonconvex objective function with Lipschitz gradient. (Since the example is unidimensional, we omit the component indices (i) if what follows.) For $k \geq 0$, let the sequence of function values and gradients be defined by

$$f_k = 0 \quad \text{and} \quad g_k = -1, \quad (5)$$

and the sequence of (potential) iterates be defined (from (2)-(4)) by

$$m_k = \beta_1 m_{k-1} + (1 - \beta_1) g_k = -1, \quad (6)$$

$$v_k = \beta_2 v_{k-1} + (1 - \beta_2) g_k^2 = 1, \quad (7)$$

$$x_{k+1} = x_k - \alpha \frac{m_k}{\sqrt{v_k}} = x_k + \alpha, \quad (8)$$

where we used (5) to derive the last equality in (6) and (7). Thus $\sum_{j=0}^k \beta^{k-j} \leq 1/(1 - \beta)$ for $\beta \in (0, 1)$ imply that

$$s_k = x_{k+1} - x_k = \alpha, \quad (9)$$

for $k \geq 0$ and x_k tends to infinity. We now show that there exists a (nonconvex) univariate function f_1 defined on \mathbb{R}^+ with Lipschitz continuous gradient such that $f_k = f(x_k) = 0$ and $g_k = \nabla_x^1 f_1(x_k) = -1$ for all $k \geq 0$. Indeed, a simple Hermite interpolation calculation based on these conditions yields that, for all $t \geq 0$,

$$f_1(t) = -(t - x_{k(t)}) + \frac{3}{s_{k(t)}} (t - x_{k(t)})^2 - \frac{2}{s_{k(t)}^2} (t - x_{k(t)})^3, \quad (10)$$

where $k(t)$ is such that $t \in [x_k, x_{k+1}]$. We may then define

$$f(t) = \begin{cases} f_1(t) & \text{if } t \geq 0, \\ -t & \text{if } t < 0, \end{cases}$$

so that $f(t)$ is well-defined on the whole of \mathbb{R} , has Lipschitz continuous gradient and is such that the ADAM algorithm (6)-(8) applied on f starting from $x_0 = 0$ generates iterates with $|g_k| = 1$ for all $k \geq 0$. We thus conclude that the ADAM algorithm fails to converge on this particular instance of problem (1). A graph of $f(t)$ for $t \in [-1, 10]$, $\beta_1 = \beta_2 = 0.9$ is shown in Figure 1. One

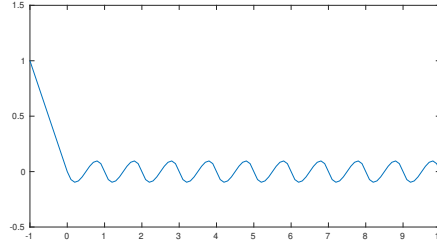


Figure 1: The shape of $f(t)$ for small values of $|t|$

also verifies that the Lipschitz constant on the interval $[x_k, x_{k+1}]$ is given by

$$L_k = \sup_{t \in (x_k, x_{k+1})} |\nabla_t^2 f(t)| = \frac{6}{s_k}$$

so that, using (9),

$$L = \max_{k \geq 0} L_k = \frac{6}{\alpha}$$

Moreover, defining $T_k(s) = f_k + g_k s$, it results from (5), [1, Theorem A.9.2], (9) and the inequalities

$$|f_{k+1} - T_k(s_k)| = s_k \leq \frac{1}{\alpha} s_k^2 \quad \text{and} \quad |g_{k+1} - \nabla_s^1 T_k(s)| = |-1 + 1| \leq \frac{1}{\alpha} s_k$$

that $f(t)$ is bounded below by a constant only depending on α . As a consequence, we see that, for any fixed $(\beta_1, \beta_2) \in [0, 1)^2$ and $\alpha > 0$, there exist unidimensional functions with Lipschitz continuous gradient whose gradient's Lipschitz constant is as small as $6/\alpha$, which is bounded below by a constant only depending on α and for which the ADAM algorithm (6)-(8) starting from $x_0 = 0$ generates iterates with constant nonzero gradients (therefore failing to converge).

Since our example is unidimensional and since ADAM is defined componentwise, the same conclusion obviously applies irrespective of n , the problem dimension. Indeed divergence in a single component implies divergence on the whole space.

Our result thus extends that of [5] in that it includes methods for arbitrary $(\beta_1, \beta_2) \in (0, 1)^2$ but fixed stepsize. Note that $|\nabla_t^1 f(t)|$ is bounded by L for all $t \in \mathbb{R}$, again at variance with the example of this reference.

Observe that our conclusions would also hold if we had fixed g_k to another negative constant (we can multiply f by this constant) or if, instead of (4), we had considered

$$[x_{k+1}]_i = [x_k]_i - \frac{\alpha [m_k]_i}{\sqrt{\epsilon + [v_k]_i^2}}, \quad \text{or} \quad [x_{k+1}]_i = [x_k]_i - \frac{\alpha [m_k]_i}{\epsilon + \sqrt{[v_k]_i^2}},$$

where ϵ is a small positive constant, but they do not apply in the more realistic situation where stepsizes $\alpha_k \rightarrow 0$ are used (as is for instance the case in [5, Proposition 1.1], where α_k is a multiple of $1/\sqrt{k}$). We finally note that we have chosen a constant zero value for f_k in order to simplify our bounds, but that it is also possible to choose $f_{k+1} > f_k$ (leading to an monotonically increasing sequence of function values) without qualitatively affecting our conclusion, although this leads to a larger value of L .

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References

- [1] C. Cartis, N. I. M. Gould, and Ph. L. Toint. Evaluation complexity of algorithms for nonconvex optimization. Number 30 in MOS-SIAM Series on Optimization. SIAM, Philadelphia, USA, June 2022.
- [2] A. Défossez, L. Bottou, F. Bach, and N. Usunier. A simple convergence proof for Adam and Adagrad. Transactions on Machine Learning Research, October 2022.
- [3] D. Kingma and J. Ba. Adam: A method for stochastic optimization. In Proceedings in the International Conference on Learning Representations (ICLR), 2015.
- [4] S. Reddi, S. Kale, and S. Kumar. On the convergence of Adam and beyond. In Proceedings in the International Conference on Learning Representations (ICLR), 2018.
- [5] Y. Zhang, C. Chen, N. Shi, R. Sun, and Z.-Q. Luo. Adam can converge without any modification on update rules. arXiv:2208.09632v5, 2022.