Convergence and Dynamical Behavior of the ADAM Algorithm for Non Convex Stochastic Optimization

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Optimization in Deep Learning

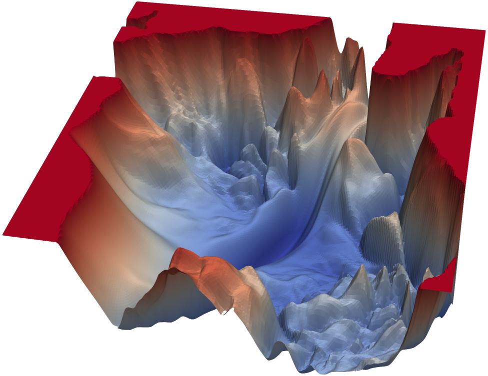

Figure 1: Visualization of a loss landscape (VGG-56 on CIFAR-10) https://www.cs.umd.edu/ tomg/projects/landscapes/

Li et al., Visualizing the Loss Landscape of Neural Nets, NeurIPS 2018

Problem statement

Problem

$$\min_x F(x) := \mathbb{E}(f(x,\xi)) \quad \text{w.r.t.} \quad x \in \mathbb{R}^d$$

Assumptions

- $f(\,.\,,\xi)$: **nonconvex** differentiable function
- $(\xi_n : n \geq 1)$: iid copies of r.v ξ revealed online

Solution ?

Stochastic Gradient Descent (SGD)

$$x_{n+1} = x_n - \gamma_n \nabla f(x_n, \xi_{n+1})$$

- Limitations
  - learning rate choice
  - common learning rate for all the coordinates

Adaptive Algorithms

standard SGD

$$x_{n+1,i} = x_{n,i} - \gamma_n \nabla f(x_n, \xi_{n+1})_i$$

$$\gamma_n := \gamma \quad \text{ou} \quad \gamma_n := \frac{1}{\sqrt{n}}, n \geq 1$$

Adaptive Algorithms

$$x_{n+1,i} = x_{n,i} - \gamma_{n,i}\, g_{n,i}$$

$$\gamma_{n,i} := \Psi(\nabla f(x_p, \xi_{p+1})_i, p \leq n)$$

ADAM Algorithm

[Kingma and Ba, 2015]

Algorithm 1 ADAM $(\gamma, \alpha, \beta, \varepsilon)$

$x_0 \in \mathbb{R}^d, m_0 = 0,\ v_0 = 0,\ \gamma > 0,\ \varepsilon > 0,\ (\alpha, \beta) \in [0,1)^2.$

for $n \geq 1$ **do**

$\quad m_n = \alpha m_{n-1} + (1-\alpha)\nabla f(x_{n-1}, \xi_n)$

$\quad v_n = \beta v_{n-1} + (1-\beta)\nabla f(x_{n-1}, \xi_n)^2$

$\quad \hat{m}_n = \frac{m_n}{1-\alpha^n}$

$\quad \hat{v}_n = \frac{v_n}{1-\beta^n}$

$\quad x_n = x_{n-1} - \frac{\gamma}{\varepsilon + \sqrt{\hat{v}_n}} \hat{m}_n$

end for

Assumptions and asymptotic regime

- Regime : **constant step size** $\gamma > 0$.

Assumptions on f

- regularity assumptions on f.
- $F : x \mapsto \mathbb{E}(f(x, \xi))$ coercive.

- Assumptions on hyperparameters: compatible with practical implementation.

From Discrete to Continuous Time

Continous Time : Dynamical System Analysis

Discrete Time : Convergence of ADAM

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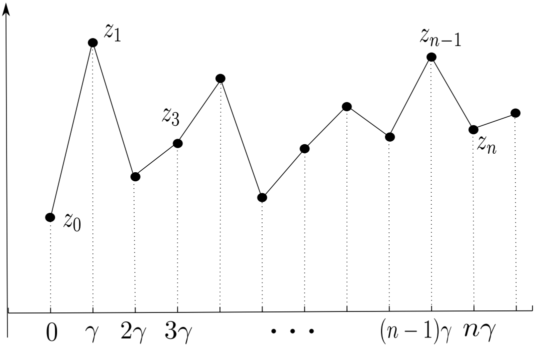
The ODE method

[Ljung, 1977, Kushner and Yin, 2003]

$\mathsf{z}^\gamma(t)$ interpolated from $z_n^\gamma = (x_n^\gamma, m_n^\gamma, v_n^\gamma)$



Towards Continuous Time

$$z_n^\gamma := z_{n-1}^\gamma + \gamma H_\gamma(n, z_{n-1}^\gamma, \xi_n)\,,$$

For all $\gamma > 0$, for all z,

$$\begin{aligned} h_\gamma(n,z) &:= \mathbb{E}(H_\gamma(n, z_{n-1}^\gamma, \xi_n)|\mathcal{F}_{n-1}) \\ \Delta_n^\gamma &:= H_\gamma(n, z_{n-1}^\gamma, \xi_n) - h_\gamma(n, z_{n-1}^\gamma) \end{aligned}$$

Decomposition in mean field + martingale noise

$$\text{For}\, \gamma > 0, \quad z_n^\gamma = z_{n-1}^\gamma + \gamma h_\gamma(n, z_{n-1}^\gamma) + \gamma \Delta_n^\gamma\,,$$

$$\frac{z_n^\gamma - z_{n-1}^\gamma}{\gamma} = h_\gamma(n, z_{n-1}^\gamma) + \Delta_n^\gamma$$

$\mathcal{F}_n = \sigma(\xi_1, \ldots, \xi_n)$

From Discrete to Continuous Time

Continous Time : Dynamical System Analysis

Discrete Time : Convergence of ADAM

Continuous Time System

similar approach to [Su et al., 2016]

Non autonomous ODE

Si $z(t) = (x(t), m(t), v(t))$,

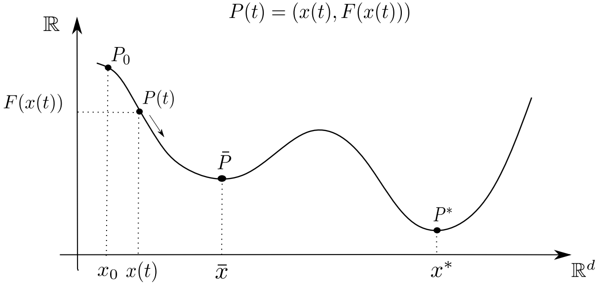
$$\dot{z}(t) = h(t, z(t)) \tag{ODE}$$

Theorem

Existence, uniqueness and boundedness of a global solution to the ODE from $(x_0, 0, 0)$.

Mechanical Interpretation - Heavy Ball with Friction

[Attouch et al., 2000, Cabot et al., 2009, Gadat et al., 2018]



- Gravity force (potentiel F).
- Force of friction of viscous type: $-\lambda \dot{x}(t)$ (damping).
- Reaction of the surface $\Sigma = Graph(F)$.

$$\ddot{x}(t) + \gamma\, \dot{x}(t) + \nabla F(x(t)) = 0$$

ADAM as a Heavy Ball with Friction (HBF)

"Generalized" HBF

$$c_1(t)\,\ddot{x}(t) + c_2(t)\,\dot{x}(t) + \nabla F(x(t)) = 0\,,$$

- **Generalized HBF :**
  - Time dependent particle mass
  - Time dependent viscosity
- **Why HBF ?**
  - 2nd vs 1st order: acceleration (even if oscillations).
  - Escaping local traps (saddle points)

Convergence to stationary points

Theorem (Convergence)

$$\lim_{t\to\infty} \mathrm{d}(x(t), \nabla F^{-1}(\{0\})) = 0\,.$$

Key argument : Lyapunov function for the ODE

- Definition :

$$V(t,z) := F(x) + \frac{1}{2}\|m\|^2_{U(t,v)^{-1}}\ .$$

- Interpretation : mechanical energy of the dynamical system
- Lemma : $t \mapsto V(t, z(t))$ is decreasing on $(0, +\infty)$.

From Discrete to Continuous Time

Continous Time : Dynamical System Analysis

Discrete Time : Convergence of ADAM

Weak convergence of the interpolated process towards the ODE solution

Techniques [Benaïm and Schreiber, 2000]

Moment assumption - Noise control

For every compact set $K \subset \mathbb{R}^d$, there exists $r_K > 0$ s.t.

$$\sup_{x \in K} \mathbb{E}(\|\nabla f(x,\xi)\|^{2+r_K}) < \infty \, .$$

Theorem

Under previous assumptions and the **moment assumption**,

$$\forall T > 0,\ \forall \delta > 0, \quad \lim_{\gamma \downarrow 0} \mathbb{P}\left(\sup_{t \in [0,T]} \|\mathsf{z}^\gamma(t) - z(t)\| > \delta \right) = 0 \, .$$

Simulations

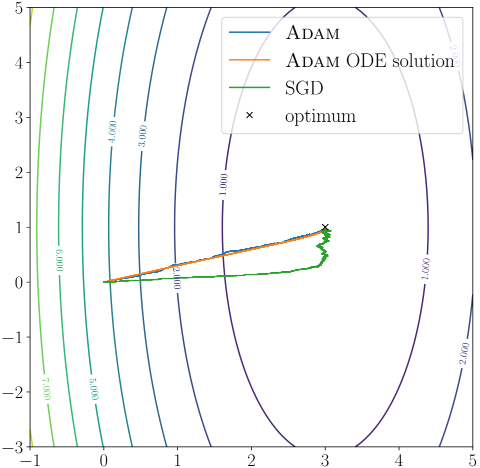


Figure 2: Convergence of ADAM and the ODE solution towards the optimum for a 2D linear regression

Long run convergence of the ADAM iterates

Techniques [Fort and Pagès, 1999, Bianchi et al., 2019]

- No a.s convergence : regime $n \to \infty$ then $\gamma \to 0$

Theorem (ergodic convergence of the ADAM iterates)

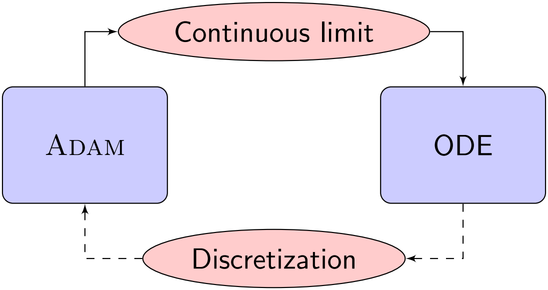
Let $x_0 \in \mathbb{R}^d$, $\gamma > 0$, $(z_n^\gamma : n \in \mathbb{N})$, $z_0^\gamma = (x_0, 0, 0)$. Under the same assumptions and :

- **Stability assumption:** $\sup_{n,\gamma} \mathbb{E}\|z_n^\gamma\| < \infty\,.$

Then, for all $\delta > 0$,

$$\lim_{\gamma \downarrow 0} \limsup_{n \to \infty} \frac{1}{n} \sum_{k=1}^{n} \mathbb{P}(\mathrm{d}(x_n^\gamma, \nabla F^{-1}(\{0\})) > \delta) = 0\,. \tag{1}$$

Conclusion



Thank you for your attention

For more details: submitted article, available on arXiv.

AB, P. Bianchi. *Convergence and Dynamical Behavior of the ADAM Algorithm for Non Convex Stochastic Optimization.*

Mean Field

where for all $t > 0$, all $z = (x, m, v)$:

$$h(t,z) = \begin{pmatrix} -\frac{(1-e^{-at})^{-1}m}{\varepsilon+\sqrt{(1-e^{-bt})^{-1}v}} \\ a(\nabla F(x) - m) \\ b(S(x) - v) \end{pmatrix}$$

$S : x \mapsto \mathbb{E}(\nabla f(x,\xi)^2)$ s.t. $\forall x \in \mathbb{R}^d$, $S(x) > 0$.

Simulations

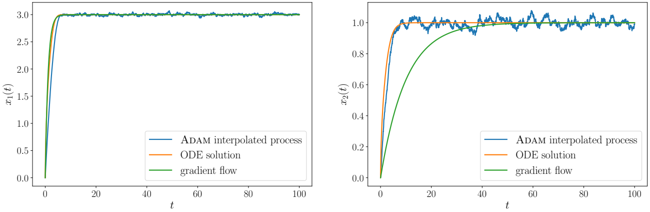


Figure 3: ADAM: interpolated process and solution to the ODE for a 2D linear regression.

2D linear regression

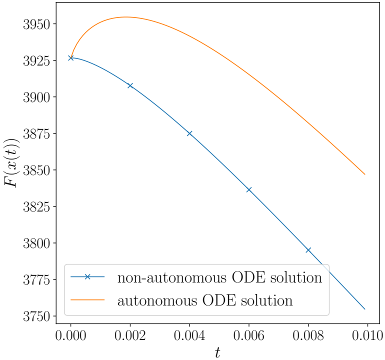
$Y = X\, x_1^* + (1 - X)\, x_2^* + \epsilon$ with $(x_1^*, x_2^*) = (3, 1)$.

$\xi = (X, Y)$ with $X \sim \mathcal{B}(p)$, $p \in (0, 1)$.

$$f(\,.\,, \xi) := \frac{1}{2}\left(\left\langle \begin{pmatrix} X \\ 1 - X \end{pmatrix}, \cdot \right\rangle - Y\right)^2.$$

Biased vs Unbiased ADAM

With debiasing steps, $F(x(t)) \leq F(x_0)$.



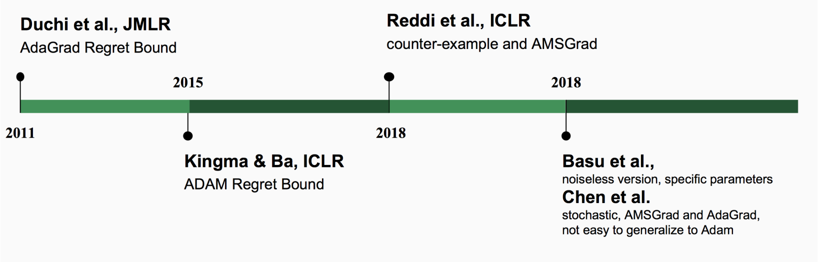
Algorithm 2 ADAM $(\gamma, \alpha, \beta, \varepsilon)$

1: $x_0 \in \mathbb{R}^d, m_0 = 0,\ v_0 = 0,\ \gamma > 0, \varepsilon > 0,\ (\alpha, \beta) \in [0, 1)^2$.
2: **for** $n \geq 1$ **do**
3: $\quad m_n = \alpha m_{n-1} + (1-\alpha)\nabla f(x_{n-1}, \xi_n)$
4: $\quad v_n = \beta v_{n-1} + (1-\beta)\nabla f(x_{n-1}, \xi_n)^2$
5: $\quad \hat{m}_n = \frac{m_n}{1-\alpha^n}$
6: $\quad \hat{v}_n = \frac{v_n}{1-\beta^n}$
7: $\quad x_n = x_{n-1} - \frac{\gamma}{\varepsilon + \sqrt{\hat{v}_n}} \hat{m}_n$
8: **end for**

Autonomous/Non autonomous ODE solutions for a 100-dimensional Stochastic Quadratic Problem

Literature review

ADAM: Theoretical results



Literature review

ADAM: theoretical results

- $\mathcal{O}(\frac{1}{\sqrt{T}})$ average regret bound in nonconvex setting.
- counter-example: average regret does not converge to 0.
- AmsGrad: variant of ADAM
- noiseless version of ADAM (deterministic f):
  - small gradient norm for some upperbounded unknown instant
  - specific values of the ADAM hyperparameters
- similar result in the stochastic setting for a general class of adaptive algorithms
  - results stated for AmsGrad and AdaGrad
  - generalization to ADAM subject to conditions which are not easy to verify.

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