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

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Outline

ADAM algorithm

From Discrete to Continuous-Time ADAM

Continuous-Time ADAM

- Existence, uniqueness, convergence
- Convergence

ADAM with decreasing stepsizes

- Almost sure convergence
- Stability
- Central Limit Theorem

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
  (+ some regularity assumptions to define F, ∇F)
- $(\xi_n : n \geq 1)$: 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 tuning
  - 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

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

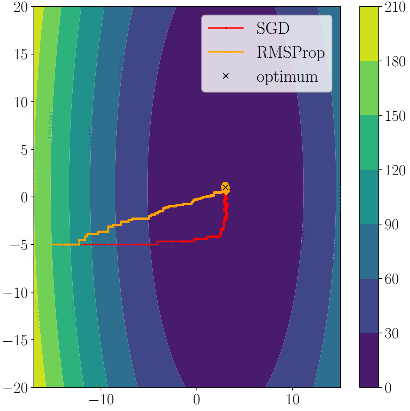
$$\gamma_{n,i} := \Psi(\nabla f(x_p, \xi_{p+1})_i, p \leq n)$$

RMSProp : coordinatewise stepsize

RMSProp

$$x_{n+1,i} = x_{n,i} - \frac{\gamma_0}{\varepsilon + \sqrt{v_{n,i}}} \nabla f(x_n, \xi_{n+1})_i$$

$$\begin{cases} x_{n+1} &= x_n - \frac{\gamma_0}{\varepsilon + \sqrt{v_n}} \nabla f(x_n, \xi_{n+1}) \\ v_{n+1} &= \beta v_n + (1-\beta) \nabla f(x_n, \xi_{n+1})^{\odot 2} \end{cases}$$

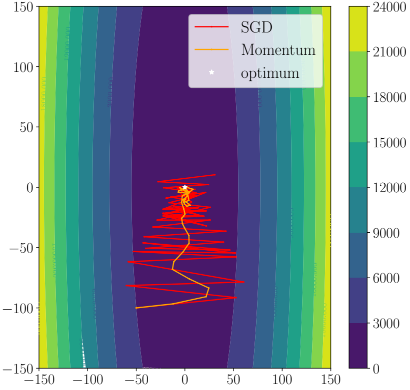


Momentum : (hoping) for acceleration

Momentum (aka Heavy Ball)

$$\begin{cases} m_n &= \alpha m_{n-1} + (1-\alpha)\nabla f(x_{n-1}, \xi_n) \\ x_{n+1} &= x_n - \gamma m_n \end{cases}$$

$$x_{n+1} = x_n - \gamma(1-\alpha)\nabla f(x_{n-1}, \xi_n) + \alpha(x_n - x_{n-1})$$



ADAM Algorithm

[Kingma and Ba, 2015]

- 51109 citations !

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

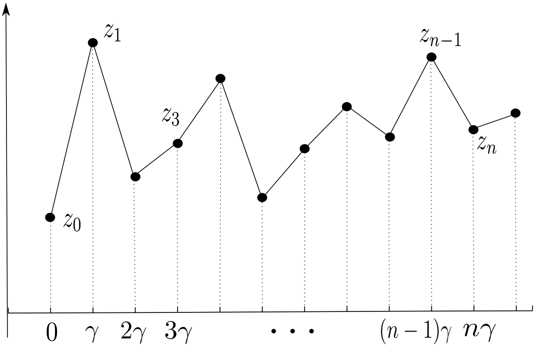
$x_0 \in \mathbb{R}^d$, $m_0 = 0$, $v_0 = 0$, $\gamma > 0$, $\varepsilon > 0$, $(\alpha, \beta) \in [0, 1)^2$.
for $n \geq 1$ **do**
  $m_n = \alpha m_{n-1} + (1 - \alpha)\nabla f(x_{n-1}, \xi_n)$
  $v_n = \beta v_{n-1} + (1 - \beta)\nabla f(x_{n-1}, \xi_n)^{\odot 2}$
  $\hat{m}_n = \frac{m_n}{1-\alpha^n}$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

I. From Discrete to Continuous-Time Adam

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,

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

Decomposition in mean field + martingale noise

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

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

Set $(\mathcal{H}_{model})$ of Assumptions

- **Model**: regularity assumptions on f (non-convex, diff., ...).
- Coercivity : $F : x \mapsto \mathbb{E}(f(x, \xi))$ coercive.
- $\forall x \in \mathbb{R}^d$, $S(x) > 0$ where $S : x \mapsto \mathbb{E}(\nabla f(x, \xi)^{\odot 2})$.
- **Hyperparameters**: verified in practice ('α,β close to 1').
- **Noise:** iid sequence (ξ_n).

II. Continuous-Time ADAM

Continuous Time System

Non autonomous ODE

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

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

Theorem

Existence, uniqueness and boundedness of a global solution to the ODE from $(x_0, 0, 0)$ under $(\mathcal{H}_{model})$.

Remark : does not stem from off-the-shelf theorems.

Convergence to stationary points

Theorem (Convergence)

Under $(\mathcal{H}_{model})$,

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

Key argument : Lyapunov function for the ODE

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

- Lemma : $t \mapsto V(t, z(t))$ is nonincreasing on $(0, +\infty)$.

- Łojasiewicz convergence rates inspired by [Haraux and Jendoubi, 2015].

III. ADAM with decreasing stepsizes

$\rightarrow$ Link between asymptotic behavior of (z_n) and ODE ?

In this Talk, ADAM with decreasing stepsizes

Algorithm 2 $\textsc{Adam}\ (((\gamma_n, \alpha_n, \beta_n) : n \in \mathbb{N}^*), \varepsilon)$.

Initialization: $x_0 \in \mathbb{R}^d$, $m_0 = 0$, $v_0 = 0$, $r_0 = \bar{r}_0 = 0$.
for $n = 1$ **to** n_{iter} **do**
  $m_n = \alpha_n m_{n-1} + (1 - \alpha_n)\nabla f(x_{n-1}, \xi_n)$
  $v_n = \beta_n v_{n-1} + (1 - \beta_n)\nabla f(x_{n-1}, \xi_n)^{\odot 2}$
  $r_n = \alpha_n r_{n-1} + (1 - \alpha_n) \longrightarrow r_n = 1 - \prod_{i=1}^{n} \alpha_i$
  $\bar{r}_n = \beta_n \bar{r}_{n-1} + (1 - \beta_n) \longrightarrow \bar{r}_n = 1 - \prod_{i=1}^{n} \beta_i$
  $\hat{m}_n = m_n / r_n$ {bias correction step}
  $\hat{v}_n = v_n / \bar{r}_n$ {bias correction step}
  $x_n = x_{n-1} - \frac{\gamma_n}{\varepsilon + \sqrt{\hat{v}_n}} \hat{m}_n$.
end for

- Define $(\mathcal{H}'_{model}) = (\mathcal{H}_{model})$ with α_n, β_n instead of α, β i.e. $\frac{1-\alpha_n}{\gamma_n} \to a$ and $\frac{1-\beta_n}{\gamma_n} \to b$.

ODE method in Stochastic Approximation

[Ljung, 1977, Kushner and Yin, 2003, Duflo, 1997, Benaïm, 1999, Borkar, 2008] ...

Robbins Monro scheme

$$\mathbf{z_{n+1}} = \mathbf{z_n} + \gamma_{\mathbf{n+1}} \underbrace{g}_{\textbf{mean field}} (\mathbf{z_n}) + \gamma_{\mathbf{n+1}} \underbrace{\eta_{n+1}}_{\textbf{noise}} + \gamma_{\mathbf{n+1}} \underbrace{b_{n+1}}_{\textbf{bias}},$$

- Noisy discretization of $\dot{\mathbf{z}}(\mathbf{t}) = \mathbf{g}(\mathbf{z}(\mathbf{t}))$.
- Informally:
  if $\gamma_n \to 0$, noise washes out and " $\lim_{n\to\infty} z_n = \lim_{t\to\infty} z(t)$".

Almost sure convergence

- RM algorithm :

$$z_{n+1} = z_n + \gamma_{n+1} \underbrace{h_\infty}_{\textit{mean field}}(z_n) + \gamma_{n+1} \underbrace{\eta_{n+1}}_{\textit{noise}} + \gamma_{n+1} \underbrace{b_{n+1}}_{\textit{bias}},$$

Assumptions ($\mathcal{H}_{as-cv}$)

- $\sum_n \gamma_n = +\infty$ and $\sum_n \gamma_n^2 < +\infty$,
- $\forall$ compact $K \subset \mathbb{R}^d$, $\sup_{x \in K} \mathbb{E}(\|\nabla f(x, \xi)\|^4) < \infty$.
- $\sup_{n \in \mathbb{N}} \|z_n\| < +\infty$ a.s.

Theorem (Almost Sure Convergence)

Under $(\mathcal{H}'_{model}) + (\mathcal{H}_{as-cv})$, w.p.1,

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

Stability

Additional assumptions ($\mathcal{H}_{stab}$)

- ∇F is Lipschitz continuous.
- $\exists C > 0 \ \forall x \in \mathbb{R}^d$, $\mathbb{E}[\|\nabla f(x,\xi)\|^2] \leq C(1 + F(x))$.

Theorem (stability)

Under $(\mathcal{H}'_{model}) + (\mathcal{H}_{as-cv}) + (\mathcal{H}_{stab})$, $(z_n = (x_n, m_n, v_n))$ satisfies

$$\sup_{n \in \mathbb{N}} \|z_n\| < \infty \quad a.s.$$

- Proof (technical) : adapt Lyapunov function to discrete time.

Towards a Central Limit Theorem

Our algorithm: $z_{n+1} = z_n + \gamma_{n+1} h_\infty(z_n) + \gamma_{n+1} b_{n+1} + \gamma_{n+1}\eta_{n+1}$,

Rescaled algorithm: $Z_{n+1} = \frac{z_{n+1} - z^*}{\sqrt{\gamma_{n+1}}}$; $\quad \gamma_n = n^{-\kappa}, \kappa \in (0, 1]$

$$\boxed{Z_{n+1} = (I + \gamma_{n+1} \underbrace{\bar{H}}_{\frac{1}{2\gamma_0}\mathbb{1}_{\kappa=1} I + \nabla h_\infty(z^*)}) Z_n + \gamma_{n+1} \bar{b}_{n+1} + \sqrt{\gamma_{n+1}}\eta_{n+1}}$$

CLT using the SDE method

[Pelletier, 1998, Duflo, 1996]

Informal Th. ([Pelletier, 1998] adapted)- Strongly disturbed algo.

$$Z_{n+1} = (I + \gamma_{n+1} \underbrace{\bar{H}}_{\textit{stable matrix}})Z_n + \gamma_{n+1}\bar{b}_{n+1} + \sqrt{\gamma_{n+1}}\eta_{n+1} \in \mathbb{R}^k$$

Under some assumptions (on (η_n) and $(\bar{b}_n)$) a.s on $\Omega_0 \in \mathcal{F}_\infty$,

$$\text{given } \Omega_0, \quad Z_n \implies \mu \,,$$

unique stationary distribution of the process

$$dX_t = \bar{H}X_t dt + \sqrt{Q} dB_t \,,$$

$$\mu \sim \mathcal{N}(0, \bar{\Sigma}) \quad \text{with } \bar{H}\bar{\Sigma} + \bar{\Sigma}\bar{H}^T = -Q \,,$$

where (B_t) Brownian, Q omitted here.

Assumptions $(\mathcal{H}_{CLT})$

- Let $x^* \in \nabla F^{-1}(\{0\})$. $\exists$ neighborhood $\mathcal{V}$ of x^* s.t.
  i) F is $\mathcal{C}^2$ on $\mathcal{V}$, and $\nabla^2 F(x^*)$ is positive definite.
  ii) S is $\mathcal{C}^1$ on $\mathcal{V}$.
- $\exists \kappa \in (0, 1]$, $\gamma_0 > 0$, s.t. $\gamma_n = \gamma_0/(n+1)^\kappa$. If $\kappa = 1$, $\gamma_0 > \frac{1}{2L}$.
- $\forall$ compact $K \subset \mathbb{R}^d$, $\exists p_K > 4$, $\sup_{x \in K} \mathbb{E}(\|\nabla f(x, \xi)\|^{p_K}) < \infty$.

Theorem (CLT)

Assume $\mathbb{P}(z_n \to z^*) > 0$.
Under $(\mathcal{H'}_{model}) + (\mathcal{H}_{CLT})$, given the event $\{z_n \to z^*\}$,

$$\frac{z_n - z^*}{\sqrt{\gamma_n}} \xrightarrow[n\to\infty]{\mathcal{D}} \mathcal{N}(0, \Sigma)\,.$$

(on $\mathbb{R}^{3d}$) with a covariance matrix Σ s.t.

$$(H + \zeta I_{3d})\,\Sigma + \Sigma\left(H^T + \zeta I_{3d}\right) = -Q\,.$$

where $\zeta := 0$ if $0 < \kappa < 1$ and $\zeta := \frac{1}{2\gamma_0}$ if $\kappa = 1$.

Asymptotic variance

- Trigonalization of

$$H := \nabla h_\infty(z^*) = \begin{pmatrix} 0 & -D & 0 \\ a\nabla^2 F(x^*) & -aI_d & 0 \\ b\nabla S(x^*) & 0 & -bI_d \end{pmatrix} \quad ; D := \mathrm{diag}\left((\varepsilon + \sqrt{S(x^*)})^{-1}\right)$$

- Influence of b, v_n? Σ_1 = limiting covariance of:

$$\begin{cases} p_{n+1} & = (1 - a\gamma_{n+1})p_n + a\gamma_{n+1} D \nabla f(x_n, \xi_{n+1}) \\ x_{n+1} & = x_n - \gamma_{n+1} p_{n+1} \,, \end{cases}$$

i.e. preconditioned stochastic heavy ball.

Contributions and future work

1. Introduction and analysis of a continuous-time ADAM.

2. Almost sure convergence of ADAM with decreasing stepsizes.

Convergence rates in discrete time? $\rightarrow$ follow-up work
Avoidance of traps?
What about the non-differentiable case?

More on : **anasbarakat.github.io**

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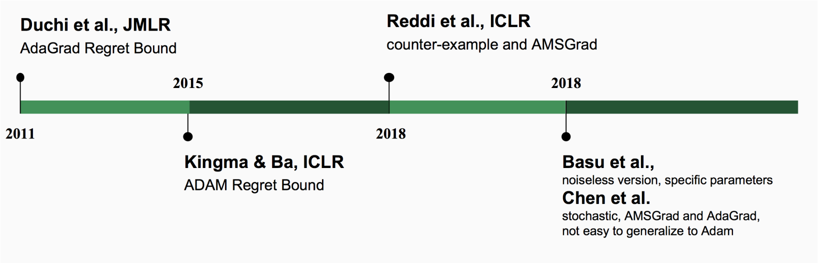
Related Work



$$\begin{cases} \dfrac{m_n - m_{n-1}}{\gamma} & = \underbrace{\dfrac{1-\alpha(\gamma)}{\gamma}}_{HYP:\, \to a \text{ as } \gamma \to 0} (\nabla F(x_{n-1}) - m_{n-1}) + \frac{1-\alpha(\gamma)}{\gamma}(\nabla f(x_{n-1}, \xi_n) - \nabla F(x_{n-1})) \\ \dfrac{v_n - v_{n-1}}{\gamma} & = \frac{1-\beta(\gamma)}{\gamma}(S(x_{n-1}) - v_{n-1}) + \frac{1-\beta(\gamma)}{\gamma}(\nabla f(x_{n-1}, \xi_n)^{\odot 2} - S(x_{n-1})) \\ \dfrac{x_n - x_{n-1}}{\gamma} & = -\frac{(1-\alpha^n)^{-1} m_n}{\varepsilon + \sqrt{(1-\beta^n)^{-1} v_n}} \end{cases}$$

$$\begin{pmatrix} \dot{x} \\ \dot{m} \\ \dot{v} \end{pmatrix} = \begin{pmatrix} -\frac{(1-e^{-at})^{-1} m}{\varepsilon + \sqrt{(1-e^{-bt})^{-1} v}} \\ a(\nabla F(x) - m) \\ b(S(x) - v) \end{pmatrix} := h(t, z) \quad \text{for } t > 0, z = (x, m, v)\,.$$

$$n = \left\lfloor \frac{t}{\gamma} \right\rfloor ; \qquad S : x \mapsto \mathbb{E}(\nabla f(x, \xi)^{\odot 2})$$

Łojasiewicz inequality

[Łojasiewicz, 1963, Attouch and Bolte, 2009]

Assumption (Łojasiewicz property)

$\forall x^* \in \nabla F^{-1}(\{0\})$, $\exists c > 0\,, \sigma > 0\,, \theta \in (0, \frac{1}{2}]$ s.t.

$$\forall x \in \mathbb{R}^d \text{ s.t } \|x - x^*\| \leq \sigma\,, \quad \|\nabla F(x)\| \geq c|F(x) - F(x^*)|^{1-\theta}\,.$$

- satisfied by broad class of functions : semialgebraic functions.

Convergence rates under Łojasiewicz property

inspired by [Haraux and Jendoubi, 2015]

Theorem (Convergence rates)

Under $(\mathcal{H}_{model})$ + Łojasiewicz inequality,

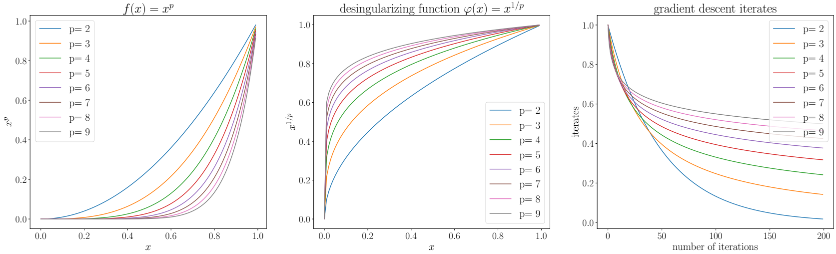
- $\exists x^* \in \nabla F^{-1}(\{0\})$ s.t. $\lim_{t\to\infty} x(t) = x^*$.
- if $\theta \in (0, \frac{1}{2}]$ is a Łojasiewicz exponent of f at x^*, $\exists C > 0$ s.t.

$$\|x(t) - x^*\| \leq C t^{-\frac{\theta}{1-2\theta}}, \quad \text{if } 0 < \theta < \frac{1}{2},$$

$$\|x(t) - x^*\| \leq C e^{-\delta t}, \quad \text{for some } \delta > 0 \text{ if } \theta = \frac{1}{2}.$$

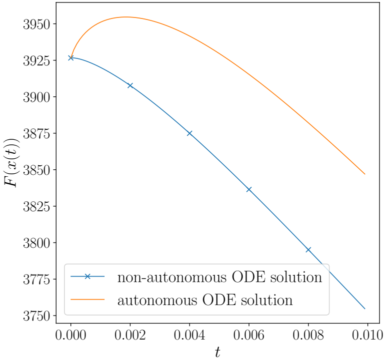
Łojasiewicz exponent and speed of convergence

- Łojasiewicz exponent : $\theta \in (0, 1]$ when $\varphi(s) = \frac{c}{\theta} s^{\theta}$.
- Basic example : slower convergence for smaller exponent $1/p$.



Biased vs Unbiased ADAM

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



Algorithm 3 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: $m_n = \alpha m_{n-1} + (1-\alpha)\nabla f(x_{n-1}, \xi_n)$
4: $v_n = \beta v_{n-1} + (1-\beta)\nabla f(x_{n-1}, \xi_n)^2$
5: $\hat{m}_n = \frac{m_n}{1-\alpha^n}$
6: $\hat{v}_n = \frac{v_n}{1-\beta^n}$
7: $x_n = x_{n-1} - \frac{\gamma}{\varepsilon + \sqrt{\hat{v}_n}} \hat{m}_n$
8: **end for**

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