Stochastic Optimization in Machine Learning: Inhomogeneity, Quantization and Acceleration

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Stochastic Approximation (SA)

$$\theta_{n+1} = \theta_n + \gamma_n H(\theta_n, X_{n+1})$$

- $\theta_n \in \mathbb{R}^d$ is the estimate at time $n$.
- $\gamma_n \in [0, \infty)$ is the step-size or learning rate at time $n$.
- $X_n \in \mathbb{R}^k$ is the new data available at time $n$.
- $H : \mathbb{R}^d \times \mathbb{R}^k \rightarrow \mathbb{R}^d$ is the update operator.

(Note: $\{\theta_n\}$, $\{X_n\}$ are random vectors; $\{\gamma_n\}$ are random scalars.)
PART I: INHOMOGENEITY

REINFORCEMENT LEARNING IN
TIME-VARYING ENVIRONMENTS

Joint work with: László Monostori (SZTAKI)
Reinforcement Learning

- Reinforcement learning (RL) is a machine learning approach to learn from interactions with an environment based on feedbacks (e.g., rewards).

- An interpretation: consider an agent acting in an uncertain environment and receiving information about the actual states and immediate costs.

- The aim is to learn an efficient behavior (control policy), such that applying this strategy minimizes the expected costs in the long run.
Applications of Reinforcement Learning

- Robot Control
- Dispatching & Scheduling
- Optimal Stopping
- Routing
- Maintenance and Repair
- Recommender Systems
- Inventory Control
- Optimal Control of Queues
- Strategic Asset Pricing
- Dynamic Options
- Insurance Risk Management
- Web System Configuration
- Bidding and Advertising
- Traffic Light Control
- Logic Games
- Communication Networks
- Dynamic Channel Allocation
- Power Grid Management
- Supply-Chain Management
- Fault Detection
- Sequential Clinical Trials
- PageRank Optimization
A (finite) **Markov Decision Process** (MDP) is characterized by

1. \( X \) is a (finite, non-empty) state space;
2. \( A \) is a (finite, non-empty) action space;
3. \( \mathcal{A} : X \to \mathcal{P}(A) \) is an action constraint function, namely, \( \mathcal{A}(x) \) is the (non-empty) set of admissible actions in \( x \in X \);
4. \( p : X \times A \to \Delta(X) \) is the transition probability function, \( p_{xy}(a) \) denotes the probability of arriving at state \( y \in X \) after taking (admissible) action \( a \in \mathcal{A}(x) \) in a state \( x \in X \);
5. \( g : X \times A \to \mathbb{R} \) is the **immediate cost** function, it is the cost (or reward) of taking action \( a \in \mathcal{A}(x) \) in state \( x \in X \).

(Note that \( \Delta(S) \) is the set of all probability distributions on \( S \); and \( \mathcal{P}(S) \) denotes the power set of set \( S \): the set of all subsets of \( S \).)
The Bellman Equation

- A (Markovian, randomized, stat.) control policy, $\pi : \mathbb{X} \rightarrow \Delta(\mathbb{A})$, is a function from states to probability distributions over actions.

- The value function, with discount factor $\alpha$, of a policy $\pi$ is

$$J^\pi(x) \overset{\text{def}}{=} \mathbb{E} \left[ \sum_{t=0}^{\infty} \alpha^t g(X_t, A_t^\pi) \right]_{X_0 = x},$$

for all $x \in \mathbb{X}$, where $A_t^\pi \sim \pi(X_t)$, $X_{t+1} \sim p(X_t, A_t)$ and $\alpha \in (0, 1)$.

- There could be many optimal policies, but they share the same optimal value function $J^*$. We typically aim at estimating $J^*$.

- The fundamental Bellman equation is $T J^* = J^*$, where

$$(T J)(x) \overset{\text{def}}{=} \min_{a \in A(x)} \left[ g(x, a) + \alpha \sum_{y \in \mathbb{X}} p(y \mid x, a) J(y) \right].$$

- Bellman operator $T$ is a contraction with Lipschitz constant $\alpha$. 

Theorem 1: assume that two MDPs differ only in their transition-probability functions, and let these two functions be $p_1$ and $p_2$. Let the corresponding optimal value functions be $J_1^*$ and $J_2^*$, then

$$
\|J_1^* - J_2^*\|_\infty \leq \frac{\alpha |X| \|g\|_\infty}{(1 - \alpha)^2} \|p_1 - p_2\|_\infty
$$

Theorem 2: assume that two MDPs differ only in the immediate-cost functions, and let these two functions be $g_1$ and $g_2$. Let the corresponding optimal value functions be $J_1^*$ and $J_2^*$, then

$$
\|J_1^* - J_2^*\|_\infty \leq \frac{1}{1 - \alpha} \|g_1 - g_2\|_\infty
$$
Theorem 3: assume that two MDPs differ only in their transition-probability functions, and let these two functions be $p_1$ and $p_2$. Let the corresponding optimal value functions be $J_1^*$ and $J_2^*$, then

$$
\|J_1^* - J_2^*\|_\infty \leq \frac{\alpha \|g\|_\infty}{(1 - \alpha)^2} \|p_1 - p_2\|_1,
$$

where $\|\cdot\|_1$ is a norm on $f : X \times A \times X \rightarrow \mathbb{R}$ type functions:

$$
\|f\|_1 = \max_{x, a} \sum_{y \in X} |f(x, a, y)|.
$$

Note: since $\forall f : \|f\|_1 \leq n \|f\|_\infty$, where $n$ is size of the state space, the bound of Theorem 3 is at least as good as that of Theorem 1.
Discount Factor Changes

Theorem 4: assume that two MDPs, $M_1$ and $M_2$, differ only in the discount factors, $\alpha_1, \alpha_2 \in (0, 1)$. Let their corresponding optimal value functions be denoted by $J_1^*$ and $J_2^*$, then

$$\|J_1^* - J_2^*\|_\infty \leq \frac{|\alpha_1 - \alpha_2|}{(1 - \alpha_1)(1 - \alpha_2)} \|g\|_\infty.$$ 

Moreover, there exists an MDP, denoted by $M_3$, such that it differs only in the immediate-cost function from $M_1$, thus its discount factor is $\alpha_1$, and it has the same optimal value function as $M_2$. The immediate-cost function of $M_3$ is

$$\hat{g}(x, a) = g(x, a) + (\alpha_2 - \alpha_1) \sum_{y \in X} p(y \mid x, a) J_2^*(y),$$

where $p$ is the transition function of all $M_i$; $g$ is the cost function of $M_1$ and $M_2$; and $J_2^*(y)$ is the optimal value function of $M_2$. 
Stochastic Optimization Perspective

– We denote the set of value functions by $\mathcal{V}$ which contains, in general, all **bounded** real-valued functions over an arbitrary set $\mathcal{X}$.

– Many (supervised and reinforcement) learning methods can be formulated as a **stochastic optimization** algorithm (SOA),

\[
V_{t+1}(x) = (1 - \gamma_t(x))V_t(x) + \gamma_t(x) \left[ (K_t V_t)(x) + W_t(x) \right],
\]

where $V_t \in \mathcal{V}$, operator $K_t : \mathcal{V} \to \mathcal{V}$ acts on value functions, $\gamma_t$ denotes the (random) stepsize and $W_t$ is the noise at time $t$.

– We will consider the case when $\{K_t\}$ are **pseudo-contractions**, e.g., Q-learning, SARSA and TD-learning can be formulated this way.

– Note that in our formulation the update operator, $K_t$, is **time-dependent**. This will be needed to handle changing dynamics.
Main Assumptions

(A1) There exits a constant \( C > 0 \) such that for all \( x \) and \( t \),

\[
\mathbb{E}\left[ W_t(x) \mid F_t \right] = 0 \quad \text{and} \quad \mathbb{E}\left[ W_t^2(x) \mid F_t \right] < C < \infty,
\]

where \( F_t = \sigma \{ V_0, \ldots, V_t, W_0, \ldots, W_{t-1}, \gamma_0, \ldots, \gamma_t \} \).

(A2) For all \( x \) and \( t \): \( \gamma_t(x) \geq 0 \) and we have with probability one

\[
\sum_{t=0}^{\infty} \gamma_t(x) = \infty \quad \text{and} \quad \sum_{t=0}^{\infty} \gamma_t^2(x) < \infty.
\]

(A3) For all \( t \), \( K_t : \mathcal{V} \to \mathcal{V} \) is a supremum norm pseudo-contraction with Lipschitz constant \( \beta_t < 1 \) and with fixed point \( V_t^* \):

\[
\forall V \in \mathcal{V} : \| K_t V - V_t^* \|_{\infty} \leq \beta_t \| V - V_t^* \|_{\infty}.
\]

Let us introduce \( \beta_0 \doteq \limsup_{t \to \infty} \beta_t \), and we assume that \( \beta_0 < 1 \).
Approximate Convergence

**Definition:** a sequence of random elements \( \{X_t\} \) from a normed space \( \kappa \)-approximates \( X \) with \( \kappa > 0 \) if for all \( \varepsilon > 0 \) there is a \( t_0 \):\[
\mathbb{P} \left( \sup_{t > t_0} \|X_t - X\| \leq \kappa \right) > 1 - \varepsilon
\]

**Theorem 5:** suppose that Assumptions (A1), (A2) and (A3) hold and let \( \{V_t\} \) be the sequence generated by a SOA. Then, for any \( V_\star, V_0 \in \mathcal{V} \), the sequence \( V_t \) \( \kappa \)-approximates function \( V_\star \) with \[
\kappa = \frac{4\varrho}{1 - \beta_0}
\] where \[
\varrho = \limsup_{t \to \infty} \|V_t^*-V_\star\|_\infty
\]

Notice that \( V_\star \) can be an arbitrary function, but, naturally, the radius of the environment of \( V_\star \), that the sequence \( \{V_t\} \) almost surely converges to, depends on \( \limsup_{t \to \infty} \|V_t^*-V_\star\|_\infty \).
A Deterministic Pathological Example

\[ k_i(v) = \begin{cases} 
    v + (1 - b_i)(v_i^* - v) & \text{if } \text{sign}(v_i^*) = \text{sign}(v) \\
    v_i^* + (v_i^* - v) + (1 - b_i)(v - v_i^*) & \text{otherwise}
\end{cases} \]

\[ v(0) = \ldots -5 -4 -3 -2 -1 0 1 2 3 4 5 \ldots \]
\[ v(1) = \ldots -5 -4 -3 -2 -1 0 1 2 3 4 5 \ldots \]
\[ v(2) = \ldots -5 -4 -3 -2 -1 0 1 2 3 4 5 \ldots \]
\[ v(3) = \ldots -5 -4 -3 -2 -1 0 1 2 3 4 5 \ldots \]
Varying Environments: \((\varepsilon, \delta)\)-MDPs

- A class of non-stationary MDPs: in this model the transition-probabilities and the immediate-costs may change over time, as long as the accumulated changes remain asymptotically bounded.

\[ \text{Definition: a tuple } \langle X, A, A, \{p_t\}_{t=1}^\infty, \{g_t\}_{t=1}^\infty, \alpha \rangle, \text{ which represents a sequence of MDPs, is called an } (\varepsilon, \delta)\text{-MDP where } \varepsilon, \delta > 0, \text{ if there exists a base MDP, } M = \langle X, A, A, p, g, \alpha \rangle, \text{ such that} \]

\[ \limsup_{t \to \infty} \|p - p_t\|_p \leq \varepsilon \quad \text{and} \quad \limsup_{t \to \infty} \|g - g_t\|_q \leq \delta, \]

where \(1 \leq p, q \leq \infty\) (henceforth, we use \(p = 1\) and \(q = \infty\)).

- The optimal value function of the base MDP, \(M\), and of the MDP at time \(t\), \(M_t\), are denoted by \(J^*\) and \(J_t^*\), respectively.
Relaxed Convergence in \((\varepsilon, \delta)\)-MDPs

Assume we have an \((\varepsilon, \delta)\)-MDP, then (using Theorems 2 and 3)

\[
\limsup_{t \to \infty} \|J^* - J^*_t\|_\infty \leq d(\varepsilon, \delta)
\]

\[
d(\varepsilon, \delta) = \frac{\alpha \varepsilon (\|g\|_\infty + \delta)}{(1 - \alpha)^2} + \frac{\delta}{1 - \alpha}
\]

where \(J^*_t\) and \(J^*\) are the optimal value functions of \(M_t\) and \(M\).

**Corollary:** consider an \((\varepsilon, \delta)\)-MDP and assume that (A1), (A2) and (A3) hold. Let \(\{V_t\}\) be the sequence generated by a SOA. Assume the fixed point of each \(K_t\) is \(J^*_t\). Then, \(V_t\) \(\kappa\)-approximates \(J^*\) with

\[
\kappa = \frac{4 d(\varepsilon, \delta)}{1 - \beta_0}
\]
Q-learning in \((\varepsilon, \delta)\)-MDPs

- Q-learning is an arch-typical model-free and off-policy RL method.
- The one-step version of Watkins’ Q-learning rule in \((\varepsilon, \delta)\)-MDPs is

\[
Q_{t+1}(x, a) \doteq (1 - \gamma_t(x, a))Q_t(x, a) + \gamma_t(x, a)(\tilde{T}_t Q_t)(x, a),
\]

\[
(\tilde{T}_t Q_t)(x, a) = g_t(x, a) + \alpha \min_{B \in A(Y)} Q_t(Y, B),
\]

where \(Y\) is a random variable generated from \((x, a)\) by simulation.
- The \(\tilde{T}_t\) operator can be rewritten in a form as follows

\[
(\tilde{T}_t Q)(x, a) = (\tilde{K}_t Q)(x, a) + \tilde{W}_t(x, a),
\]

where \(\tilde{W}_t(x, a)\) is a noise with zero mean and finite variance, and

\[
(\tilde{K}_t Q)(x, a) = g_t(x, a) + \alpha \sum_{y \in X} p_t(y \mid x, a) \min_{b \in A(y)} Q(y, b).
\]
Q-learning in $(\varepsilon, \delta)$-MDPs

- $W_t$ has zero mean and finite variance $\Rightarrow$ (A1) is satisfied.
- Each $\tilde{K}_t$ operator is an $\alpha$ contraction $\Rightarrow$ (A3) holds.
- Thus, (A2) $\Rightarrow \{Q_t\}$ generated by Q-learning $\kappa$-approximates $Q^*$, the optimal action-value function, with $\kappa = 4 \frac{d(\varepsilon, \delta)}{1 - \alpha}$.
- Similarly guarantees can be obtained for other RL methods, e.g., TD($\lambda$) and asynchronous value iteration working in $(\varepsilon, \delta)$-MDPs.

Lemma: assume we have two MDPs which differ only in the transition-probability functions or only in the immediate-cost functions or only in the discount factors. Let the corresponding optimal action-value functions be $Q_1^*$ and $Q_2^*$, respectively. Then the bounds for $\|J_1^* - J_2^*\|_\infty$ of Theorems 2, 3 and 4 are also bounds for the optimal action-value function changes $\|Q_1^* - Q_2^*\|_\infty$. 

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Summary of Part I: Inhomogeneity

- The optimal (state and action) value functions of discounted MDPs Lipschitz continuously depend on the transition-probability and the immediate-cost functions. Changes in the discount factor can be traced back to changes in the immediate-costs.

- In \((\varepsilon, \delta)\)-MDPs these functions may vary over time, provided that the accumulated changes remain asymptotically bounded.

- A convergence theorem for stochastic optimization algorithms with time-dependent pseudo-contraction updates was given, which guarantees convergence to an environment of a target function.

- These results can be combined to deduce convergence theorems for reinforcement learning algorithms working in changing MDPs, which was demonstrated by studying Q-learning in \((\varepsilon, \delta)\)-MDPs.
Part II: Quantization

Recursive Estimation of ARX Systems Using Binary Sensors

Joint work with: Erik Weyer (University of Melbourne)
Binary Identification of ARX Systems

- Problem: estimating ARX systems observed via binary sensors.
- Previous (textbook) solutions typically assumed fully known noise characteristics and that the input signal can be chosen by the user.
- We try to reduce the assumptions on the noise and the input.
- Full knowledge of the noise distribution is not needed.
- The input is only assumed to be observed and not controlled.
- But, the threshold of the sensor must be controlled (which approach has similarities with dithering signal based solutions).
- Here, two recursive identification algorithms are proposed.
- Algorithm I: FIR approximation; which is strongly consistent.
- Algorithm II: simultaneous state and parameter estimation.
Problem Setting

– We observe an ARX (autoregressive exogenous) system via a binary sensor (where \( I \) denotes an indicator function):

\[
X_t = \sum_{i=1}^{p} a_i^* X_{t-i} + \sum_{i=1}^{q} b_i^* U_{t-i} + N_t,
\]

\[
Y_t = I(X_t \leq C_t),
\]

where \( X_t \) — state, \( U_t \) — input, \( N_t \) — noise (at time \( t \)).

– The thresholds of the binary sensor, \( \{C_t\} \), can be controlled.

– Data: the inputs \( \{U_t\} \) and the binary outputs \( \{Y_t\} \) are observed.

– Aim: to estimate (identify) \( \theta^* = (a_1^*, \ldots, a_p^*, b_1^*, \ldots, b_q^*)^T \in \mathbb{R}^{p+q} \)
System Assumptions

- The noises $\{N_t\}$ are i.i.d., continuous, zero mean, zero median, $E[N_t^2] < \infty$, and have a continuous and positive density at zero.
- The inputs $\{U_t\}$ are i.i.d., zero mean, and $0 < E[U_t^2] < \infty$.
- The input $\{U_t\}$ and the noise $\{N_t\}$ sequences are independent.
- The system is stable, i.e., the roots of $A^*(z)$ lie strictly inside the unit circle; and the transfer function $B^*(z)/A^*(z)$ is irreducible,

$$A^*(z) = 1 - a_1^*z^{-1} - a_2^*z^{-2} - \cdots - a_p^*z^{-p},$$

$$B^*(z) = b_1^*z^{-1} + b_2^*z^{-2} + \cdots + b_q^*z^{-q},$$

where $z^{-1}$ is the backward shift operator (recall, $z^{-i}x_t \equiv x_{t-i}$).
- The orders (of polynomials $A^*$ and $B^*$) $p$ and $q$ are known.
Adjustable Thresholds \sim Dithering

– The binary output can be rewritten as

\[ Y_t = \mathbb{1}(\varphi_t^T \theta^* + N_t \leq C_t) = \mathbb{1}(\varphi_t^T \theta^* + N_t - C_t \leq 0), \]

where \( \varphi_t = (X_{t-1}, \ldots, X_{t-p}, U_{t-1}, \ldots, U_{t-q}) \) is the regressor.

– Therefore, choosing the threshold is similar to dithering:
General Form of the Algorithms

- The general form of both proposed algorithms is

\[
\hat{\theta}_{t+1} = \Pi_{M_{\mu(t)}} \left[ \hat{\theta}_t + \alpha_t \hat{\varphi}_t \left( 1 - 2 \mathbb{I}(X_t \leq \hat{\varphi}_t^T \hat{\theta}_t) \right) \right],
\]

where \( \hat{\varphi}_t \) is a regressor defined differently in the two algorithms, \( \{\alpha_t\} \) are the step-sizes and \( \Pi_{M_{\mu(t)}} \) is a sequence of projections.

- As we assumed that \( N_t \) is continuous, we (almost surely) have

\[
1 - 2 \mathbb{I}(X_t \leq \hat{\varphi}_t^T \hat{\theta}_t) = \text{sign}(X_t - \hat{\varphi}_t^T \hat{\theta}_t).
\]

- Therefore, the above algorithm will behave almost surely as

\[
\hat{\theta}_{t+1} = \Pi_{M_{\mu(t)}} \left[ \hat{\theta}_t + \alpha_t \hat{\varphi}_t \text{sign}(X_t - \hat{\varphi}_t^T \hat{\theta}_t) \right],
\]

which is a sign-error method with expanding truncation bounds.
Step-Size Assumptions

– Typical step-size assumption of stochastic optimization algorithms

\[
\sum_{t=0}^{\infty} \alpha_t = \infty,
\]

\[
\sum_{t=0}^{\infty} \alpha_t^2 < \infty,
\]

\[\forall t : \alpha_t \geq 0.\]

– Henceforth, we will simply assume that for all \( t \) we use

\[
\alpha_t = \frac{1}{t + 1}.
\]
Expanding Truncation Bounds

- Let \( \{M_t\} \) be a sequence of (strictly) monotone increasing positive real numbers with \( M_t \to \infty \) as \( t \to \infty \).

- Let \( \mathbb{I}(\cdot) \) be the indicator function and define \( \mu(t) \) and \( \Delta \hat{\theta}_i \) as

\[
\mu(t) = \sum_{i=1}^{t-1} \mathbb{I}(|\hat{\theta}_i + \Delta \hat{\theta}_i| > M_{\mu(i)}),
\]

\[
\Delta \hat{\theta}_i = \alpha_i \hat{\varphi}_i (1 - 2 \mathbb{I}(X_i \leq \hat{\varphi}_i^T \hat{\theta}_i)).
\]

- Given a positive real \( M \), projection \( \Pi_M \) is

\[
\Pi_M(x) = \begin{cases} 
  x & \text{if } \|x\| \leq M, \\
  0 & \text{otherwise.}
\end{cases}
\]
Algorithm I: FIR Approximation

- Using impulse responses, \((c_i^*)_{i=1}^{\infty}\) and \((d_i^*)_{i=0}^{\infty}\), we have

\[
X_t = \sum_{i=1}^{\infty} c_i^* U_{t-1} + \sum_{i=0}^{\infty} d_i^* N_{t-i},
\]

- Let’s approximate our ARX system with an FIR with order \(p + q\)

\[
X_t = \bar{\varphi}_t^T \bar{\theta}^* + W_t,
\]

\[
\bar{\varphi}_t = (U_{t-1}, \ldots, U_{t-p-q})^T, \quad \bar{\theta}^* = (c_1^*, \ldots, c_{p+q}^*)^T.
\]

- And \(W_t\) is simply the unmodelled part of the system

\[
W_t = \sum_{i=p+q+1}^{\infty} c_i^* U_{t-i} + \sum_{i=0}^{\infty} d_i^* N_{t-i}.
\]
Algorithm I: FIR Approximation

- If we can estimate $\bar{\theta}^*$, we can also estimate the true $\theta^*$.
- There is a function $f$, which we use for post processing, such that
  \[ \theta^* = f(\bar{\theta}^*), \]
- Algorithm I is defined by using $\hat{\varphi}_t = \bar{\varphi}_t$ in the General Algorithm.

**Theorem: Strong Consistency.** Let $(\hat{\theta}_t)_{t=0}^\infty$ be the sequence generated by Algorithm I. Then, under the given assumptions, $f(\hat{\theta}_t)$ converges (a.s.) to $\theta^*$, as $t \to \infty$, from any $\hat{\theta}_0 \in \mathbb{R}^{p+q}$.

- Moreover, one can show that $\sqrt{t} (\hat{\theta}_t - \bar{\theta}^*)$ is approximately normal.
Algorithm II: Simultaneous Estimation

- Main idea: to achieve a direct estimate of $\theta^*$ by simultaneously maintaining estimates for both $\hat{X}_t$ and $\hat{\theta}_t$, at time $t$.
- The sequence of output estimates can be defined as

$$
\hat{X}_t = \begin{cases} 
\sum_{i=1}^{p} \hat{a}_{t,i} \hat{X}_{t-1} + \sum_{i=1}^{q} \hat{b}_{t,i} U_{t-i} & \text{if } t \geq 0 \\
0 & \text{otherwise},
\end{cases}
$$

where $(\hat{a}_{t,i})_{i=1}^{p}$ and $(\hat{b}_{t,i})_{i=1}^{q}$ are estimates of the true parameters.
- Algorithm II: is defined by setting the General Algorithm as

$$
\hat{\varphi}_t \equiv (\hat{X}_{t-1}, \ldots, \hat{X}_{t-p}, U_{t-1}, \ldots, U_{t-q})^T,
\hat{\theta}_t \equiv (\hat{a}_{t,1}, \ldots, \hat{a}_{t,p}, \hat{b}_{t,1}, \ldots, \hat{b}_{t,q})^T.
$$
Simulation Experiment: ARX(2, 2)

Figure: Recursive estimation with Algorithm I
Simulation Experiment: ARX(2, 2)

Figure: Recursive estimation with Algorithm II
Summary of Part II: Quantization

- Two recursive identification algorithms have been proposed for identifying ARX systems observed via a binary sensor.
- These algorithms neither assume the knowledge of the noise distributions, nor assume that the input signal can be chosen.
- However, we should be able to control the threshold of the sensor.
- This assumption is similar to allowing a dithering signal.
- Both algorithms are special cases of our General Algorithm that can be reformulated as a sign-error method (it is also equivalent to a stochastic gradient descent algorithm based on L1 error).
- Algorithm I: FIR approximation; which is strongly consistent.
- Algorithm II: simultaneous state and parameter estimation.
- Experimental results demonstrated that both algorithms efficiently approximated the parameters of an ARX(2,2) system.
Part III: Acceleration

Asymptotic Analysis of the LMS Algorithm with Momentum

Joint work with: László Gerencsér (SZTAKI) and Sotirios Sabanis (University of Edinburgh)
Introduction

- **Stochastic gradient descent (SGD)** methods are popular stochastic approximation (SA) algorithms applied in a wide variety of fields.
- Here, we focus on the special case of **least mean square (LMS)**.
- Polyak’s **momentum** is an acceleration technique for gradient methods which has several advantages for deterministic problems.
- K. Yuan, B. Ying and A. H. Sayed (2016) argued that in the stochastic case it is “equivalent” to standard SGD, assuming fixed gains, strongly convex functions and martingale difference noises.
- For LMS, they assumed independent noises to ensure this.
- Here, we provide a significantly simpler asymptotic analysis of LMS with momentum for stationary, ergodic and mixing signals.
- We present weak convergence results and explore the trade-off between the rate of convergence and the asymptotic covariance.
Stochastic Gradient Descent

– We want to minimize an unknown function, \( f : \mathbb{R}^d \rightarrow \mathbb{R} \), based only on noisy queries about its gradient, \( \nabla f \), at selected points.

Stochastic Gradient Descent (SGD)

\[
\theta_{n+1} = \theta_n + \mu (-\nabla_{\theta} f(\theta_n) + \varepsilon_n)
\]

– Polyak’s heavy-ball or momentum method is defined as

SGD with Momentum Acceleration

\[
\theta_{n+1} = \theta_n + \mu (-\nabla_{\theta} f(\theta_n) + \varepsilon_n) + \gamma (\theta_n - \theta_{n-1})
\]

– The added term acts both as a smoother and an accelerator.
  (The extra momentum dampens oscillations and helps us getting through narrow valleys, small humps and local minima.)
Mean-Square Optimal Linear Filter

- [C0] Assume we observe a (strictly) stationary and ergodic stochastic process consisting input-output pairs \( \{(x_t, y_t)\} \), where regressor (input) \( x_t \) is \( \mathbb{R}^d \)-valued, while output \( y_t \) is \( \mathbb{R} \)-valued.

- We want to find the mean-square optimal linear filter coefficients \( \theta^* \).

\[
\theta^* \doteq \arg \min_{\theta \in \mathbb{R}^d} \mathbb{E}\left[ \frac{1}{2} (y_n - x_n^T \theta)^2 \right]
\]

- Using \( R_* \doteq \mathbb{E}[x_n x_n^T] \) and \( b \doteq \mathbb{E}[x_n y_n] \), the optimal solution is

Wiener-Hopf Equation

\[
R_* \theta^* = b \quad \Rightarrow \quad \theta^* = R_*^{-1} b
\]

- [C1] Assume that \( R_* \) is non-singular, thus, \( \theta^* \) is uniquely defined.
Least Mean Square

- The least mean square (LMS) algorithm is an SGD method

\[
\theta_{n+1} = \theta_n + \mu x_{n+1} \left( y_{n+1} - x_{n+1}^T \theta_n \right)
\]

with \( \mu > 0 \) and some constant (non-random) initial condition \( \theta_0 \).

- Introducing the observation and (coefficient) estimation errors as

\[
\nu_n = y_n - x_n^T \theta^*
\]

and

\[
\Delta_n = \theta_n - \theta^*
\]

the estimation error process, \( \{\Delta_n\} \), follows the dynamics

\[
\Delta_{n+1} = \Delta_n - \mu x_{n+1} x_{n+1}^T \Delta_n + \mu x_{n+1} \nu_{n+1}
\]

with \( \Delta_0 = \theta_0 - \theta^* \). Note that \( \mathbb{E} [x_n \nu_n] = 0 \) for all \( n \geq 0 \).
The Associated ODE

- A standard tool for the analysis of SA methods is the associated ordinary differential equation (ODE). In the LMS case (for \( t \geq 0 \))

\[
\frac{d}{dt} \bar{\theta}_t = h(\bar{\theta}(t)) = b - R^*\bar{\theta}_t \quad \text{with} \quad \bar{\theta}_0 = \theta_0
\]

where \( h(\theta) = \mathbb{E} [ x_{n+1} (y_{n+1} - x_{n+1}^T \theta) ] \) is the mean update for \( \theta \).

- A piecewise constant extension of \( \{ \theta_n \} \) is defined as \( \theta_c^t = \theta_{[t]} \), (note that here \( [t] \) denotes the integer part of \( t \)).

- LMS is modified by taking a truncation domain \( D \), where \( D \) is the interior of a compact set; then we apply the stopping time

\[
\tau = \inf \{ t : \theta_c^t \notin D \}
\]

- \([C2]\) We assume that the truncation domain is such that the solution of the ODE defined above does not leave \( D \).
The Error of the ODE

- Let us define the following error processes for the mean ODE
  \[ \tilde{\theta}_n \equiv \theta_n - \bar{\theta}_n \quad \text{and} \quad \tilde{\theta}_c^t \equiv \theta_c^t - \bar{\theta}_t \]

- The normalized and time-scaled version of the ODE error is
  \[
  V_t(\mu) \doteq \mu^{-1/2} \tilde{\theta}_{(t \wedge \tau) / \mu} = \mu^{-1/2} \tilde{\theta}_{c(t \wedge \tau) / \mu}
  \]

- We will also need the asymptotic covariance matrices of the empirical means of the centered correction terms, given by
  \[
  S(\theta) \doteq \sum_{k=-\infty}^{+\infty} \mathbb{E} \left[ (H_k(\theta) - h(\theta))(H_0(\theta) - h(\theta))^T \right]
  \]
  where \( H_n(\theta) \doteq x_n(y_n - x_n^T \theta) \), which series converges, for example, under various mixing conditions (this will be ensured by \([C3]\)).
Weak Convergence for LMS

- [C3] We assume that the process defined by

\[ L_t(\mu) = \sum_{n=0}^{[t/\mu]-1} \left( H_n(\bar{\theta}_n) - h(\bar{\theta}_n) \right) \sqrt{\mu} \]

converges weakly, as \( \mu \to 0 \), to a time-inhomogeneous zero-mean Brownian motion \( \{L_t\} \) with local covariances \( \{S(\bar{\theta}_t)\} \).

Theorem 1: Weak Convergence for LMS

Under conditions C0, C1, C2 and C3, process \( \{V_t(\mu)\} \) converges weakly, as \( \mu \to 0 \), to a process \( \{Z_t\} \) satisfying the following linear stochastic differential equation (SDE), for \( t \geq 0 \), with \( Z_0 = 0 \),

\[ dZ_t = -R^*Z_t \, dt + S^{1/2}(\bar{\theta}_t) \, dW_t \]

where \( \{W_t\} \) is a standard Brownian motion in \( \mathbb{R}^d \).
### Momentum LMS

**LMS with Momentum Acceleration**

\[ \theta_{n+1} = \theta_n + \mu x_{n+1} (y_{n+1} - x_{n+1}^T \theta_n) + \gamma (\theta_n - \theta_{n-1}) \]

with \( \mu > 0 \), \( 1 > \gamma > 0 \), and some non-random \( \theta_0 = \theta_{-1} \).

- The filter coefficient errors now follow a 2nd order dynamics

\[ \Delta_{n+1} = \Delta_n - \mu x_{n+1} x_{n+1}^T \Delta_n + \mu x_{n+1} v_{n+1} + \gamma (\Delta_n - \Delta_{n-1}) \]

with \( \Delta_0 = \Delta_{-1} \) (recall that \( \Delta_n \doteq \theta_n - \theta^* \) and \( v_n \doteq y_n - x_n^T \theta^* \)).

- To handle higher-order dynamics, we can use a state-vector,

\[ U_n \doteq \begin{bmatrix} \Delta_n \\ \Delta_{n-1} \end{bmatrix} \]
State-Space Form for Momentum LMS

Using $U_n \doteq [\Delta_n, \Delta_{n-1}]^T$, the state-space dynamics becomes

$$U_{n+1} = U_n + A_{n+1}U_n + \mu W_{n+1},$$

$$A_{n+1} \doteq \begin{bmatrix} \gamma/I - \mu \cdot x_{n+1}x_{n+1}^T & -\gamma/I \\ I & -I \end{bmatrix}, \quad W_{n+1} \doteq \begin{bmatrix} x_{n+1}v_{n+1} \\ 0 \end{bmatrix}$$

This, however, does not have the canonical form of SA methods.

We apply a state-space transformation by Yuan, Ying and Sayed,

$$T = T(\gamma) = \frac{1}{1-\gamma} \begin{bmatrix} I & -\gamma/I \\ I & -I \end{bmatrix}$$

$$T^{-1} = T^{-1}(\gamma) = \begin{bmatrix} I & -\gamma/I \\ I & -I \end{bmatrix}$$
Transformed State-Space Dynamics

- To get a standard SA form, we also need to synchronize $\gamma$ and $\mu$,
  \[
  \frac{\mu}{1 - \gamma} = c (1 - \gamma) \quad \text{leading to} \quad \mu = c (1 - \gamma)^2.
  \]
  with some fixed constant (hyper-parameter) $c > 0$.
- After applying $T$, the transformed dynamics becomes an (almost) canonical SA recursion with the fixed gain $\lambda = 1 - \gamma$ as follows:

\[
\tilde{U}_{n+1} = \tilde{U}_n + \lambda \left( \left[ \tilde{B}_{n+1} + \lambda \tilde{D}_{n+1} \right] \tilde{U}_n + \tilde{W}_{n+1} \right)
\]

\[
\tilde{B}_n = \begin{bmatrix}
0 & 0 \\
0 & -I
\end{bmatrix} + c \begin{bmatrix}
-1 & 1 \\
-1 & 1
\end{bmatrix} \otimes x_n x_n^T,
\]

\[
\tilde{D}_n = c \begin{bmatrix}
0 & -1 \\
0 & -1
\end{bmatrix} \otimes x_n x_n^T, \quad \tilde{W}_n = c \begin{bmatrix}
x_n v_n \\
x_n v_n
\end{bmatrix}.
\]
The Associated ODE for Momentum LMS

– Let us introduce the notations

\[ \bar{H}_n(\bar{U}) \doteq (\bar{B}_n + \lambda \bar{D}_n)\bar{U} + \bar{W}_n \]

\[ h(\bar{U}) \doteq \mathbb{E}[\bar{H}_n(\bar{U})] = \bar{B}_\lambda \bar{U} \]

\[ \bar{B}_\lambda \doteq \mathbb{E}[\bar{B}_n + \lambda \bar{D}_n] = \begin{bmatrix} 0 & 0 \\ 0 & -1 \end{bmatrix} + c \begin{bmatrix} -1 & 1 - \lambda \\ -1 & 1 - \lambda \end{bmatrix} \otimes R^* \]

Then, the associated ODE takes the form, with \( \bar{U}_0 = \bar{U}_0 \),

\[ \frac{d}{dt} \bar{U}_t = \bar{h}(\bar{U}_t) = \bar{B}_\lambda \bar{U}_t \]

– The solution for the limit when \( \lambda \downarrow 0 \) is denoted by \( \bar{U}_t^* \).

– Lemma: If \( \lambda \) is sufficiently small, then \( \bar{B}_\lambda \) is stable.
The ODE Error for Momentum LMS

- [C2’] We again introduce a truncation domain, \( \bar{D} \), as an interior of a compact set, and assume that the ODE does not leave \( \bar{D} \).
- We set a stopping time for leaving the domain
  \[ \bar{\tau} \doteq \inf \{ n : \bar{U}_n \notin \bar{D} \} \]
- And define the error process, for \( n \geq 0 \), as
  \[ \tilde{\bar{U}}_n \doteq \bar{U}_n - \bar{\bar{U}}_n \]
- Finally, the normalized and time-scaled error process is
  \[ \tilde{V}_t(\lambda) \doteq \lambda^{-1/2} \tilde{\bar{U}}_{[(t \wedge \bar{\tau})/\lambda]} \]
- However, the weak convergence theorems for SA methods cannot be directly applied, because there is an extra \( \lambda \) term in the update.
Approximation by Standard SA Recursion

- We will **approximate** the original process by (of course, $\bar{U}_0^* = \bar{U}_0$)

$$\bar{U}_{n+1}^* = \bar{U}_n^* + \lambda \left( \bar{B}_{n+1} \bar{U}_n^* + \bar{W}_{n+1} \right)$$

- Using the same steps as before, we can define the **normalized** and **time-scaled** ODE error process for the approximation as

$$\bar{V}_t^*(\lambda) \doteq \lambda^{-1/2} \bar{U}_{[(t \wedge \bar{\tau})/\lambda]}$$

where the **truncation domain** $\bar{D}^*$, for $\bar{\tau}^*$, is such that $\bar{D} \subseteq \text{int}(\bar{D}^*)$.

- [CW] Assume $\bar{V}_t(\lambda) - \bar{V}_t^*(\lambda)$ converges weakly to 0, as $\lambda \to 0$ (for Momentum LMS, this could be proved based on linearity).

- Thus, **weak convergence** results can be applied to the approximate process, $\{\bar{V}_t^*(\lambda)\}$, and the results will **carry over** to $\{\bar{V}_t(\lambda)\}$. 
Local Covariances for Momentum LMS

– The asymptotic covariance matrices of the empirical means of the centered correction terms are (under reasonable conditions)

\[ \bar{S}(\bar{U}) = \sum_{k=-\infty}^{+\infty} \mathbb{E} \left[ (H_k^*(\bar{U}) - \bar{h}^*(\bar{U}))(H_0^*(\bar{U}) - \bar{h}^*(\bar{U}))^T \right] \]

where \( H_k^* \) and \( h^* \) denote the limit of \( H_k \) and \( h \) as \( \lambda \downarrow 0 \).

– [C3’] We assume that the process defined by

\[ \bar{L}_t(\lambda) = \sum_{n=0}^{[t/\lambda] - 1} \left( H_n^*(\bar{U}_{\lambda n}) - \bar{h}^*(\bar{U}_{\lambda n}) \right) \sqrt{\lambda} \]

converges weakly, as \( \lambda \to 0 \), to a time-inhomogeneous zero-mean Brownian motion \( \{ \bar{L}_t \} \) with local covariance matrices \( \{ \bar{S}(\bar{U}_t^*) \} \).
**Theorem 2: Weak Convergence for Momentum LMS**

Under conditions C0, C1, C2', C3' and CW, process \( \{\bar{V}_t(\lambda)\} \) converges weakly, as \( \lambda \to 0 \), to a process \( \{\bar{Z}_t\} \) satisfying the following linear stochastic differential equation (SDE),

\[
d\bar{Z}_t = \bar{B}_* \bar{Z}_t \, dt + \bar{S}^{1/2} (\bar{U}_t^*) \, d\bar{W}_t
\]

for \( t \geq 0 \), with initial condition \( \bar{Z}_0 = 0 \), where \( \{\bar{W}_t\} \) is a standard Brownian motion in \( \mathbb{R}^{2d} \) and matrix \( \bar{B}_* \) is defined as

\[
\bar{B}_* = \lim_{\lambda \downarrow 0} \bar{B}_\lambda = \begin{bmatrix} 0 & 0 \\ 0 & -1 \end{bmatrix} + c \begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix} \otimes R^* \]
Lyapunov Equation for Momentum LMS

- The asymptotic covariance matrix of \( \{ \tilde{Z}_t \} \), denoted by \( \tilde{P} \), satisfies the Lyapunov equation (it is a transformed process)

\[
\tilde{B}^* \tilde{P} + \tilde{P} \tilde{B}^*_T + \tilde{S} = 0
\]

- Lemma: the solution of this Lyapunov equation is

\[
\tilde{P} = \frac{c}{2} \begin{bmatrix} c S + 2P_0 & c S \\ c S & c S \end{bmatrix}
\]

where \( P_0 \) is the asymptotic covariance of the weak limit of LMS.

- Let us denote the asymptotic covariance matrix of \( \{ T_1^+ \tilde{Z}_t \} \) by \( P \), where \( T_1^+ \) is the limit of \( T^{-1}(\gamma) \) as \( \gamma \to 1 \) (or \( \lambda \to 0 \)). Then,

\[
P = T_1^+ \tilde{P} (T_1^+)^T = c \begin{bmatrix} P_0 & P_0 \\ P_0 & P_0 \end{bmatrix}
\]
Comparing LMS with and without Momentum

Theorem 3: Asymptotic Covariance of Momentum LMS

Assume C0, C1, C2, C2', C3, C3', CW and that the weak convergences carry over to $\mathcal{N}(0, P_0)$ and $\mathcal{N}(0, P)$, as $t \to \infty$, in the case of plain and Momentum LMS methods, respectively.

Then, the covariance (sub)matrix of the asymptotic distribution associated with LMS with momentum is $c \cdot P_0$, where $P_0$ is the corresponding covariance of plain LMS and $c = \mu/(1 - \gamma)^2$.

- If $c = 1$, then the two asymptotic covariances are the same.
- But, the convergence rates are quite different, as the normalization is $\mu^{-1/2}$ for LMS and $\lambda^{-1/2}$ for Momentum LMS with $\lambda = \sqrt{\mu}$.
- Decreasing $c$ decreases the asymptotic covariance matrix, but it also decreases the convergence rate, and vice versa, $\lambda = \sqrt{\mu/c}$.
Summary of Part III: Acceleration

– We have analyzed the effect of momentum acceleration on the LMS algorithm, as a special case of SGD with fixed gain.
– Momentum acceleration has many known advantages in the deterministic case, but in a stochastic setting it is found to be “equivalent” to standard SGD by Yuan, Ying and Sayed (2016).
– However, for fixed-gain LMS, they only showed this equivalence for the (restrictive) special case of independent observations.
– Here, we provided a simpler asymptotic analysis of LMS with momentum acceleration for stationary, ergodic and mixing signals.
– We presented weak convergence results and explored the trade-off between the rate of convergence and the asymptotic covariance.
– The approach can be generalized to a wide range of SA methods.
Thank you for your attention!

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