

Asymptotic behavior of stochastic algorithms with statistical applications Part 2

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1 The Robbins-Monro algorithm

- Introduction.
- Almost sure convergence.
- Asymptotic normality.

2 The Kiefer-Wolfowitz algorithm

- Introduction.
- Almost sure convergence.
- Asymptotic normality.

3 Acceleration by averaging

- Introduction.
- Almost sure convergence.
- Asymptotic normality.

Outline

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Stochastic approximation.



Herbert Robbins

Stochastic approximation.

Let f be an **unknown function** from \mathbb{R}^d to \mathbb{R}^d .

Goal

→ For a **given vector** α of \mathbb{R}^d , find a vector \mathbf{x}^* which satisfies

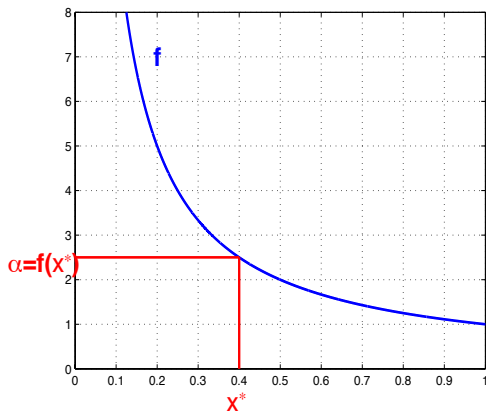
$$f(\mathbf{x}^*) = \alpha.$$

We will assume in all the sequel that for all $n \geq 1$, we can compute X_1, \dots, X_n of \mathbb{R}^d and we can find Y_{n+1} of \mathbb{R}^d such that

$$\mathbb{E}[Y_{n+1} | \mathcal{F}_n] = f(X_n)$$

where $\mathcal{F}_n = \sigma(X_1, \dots, X_n)$.

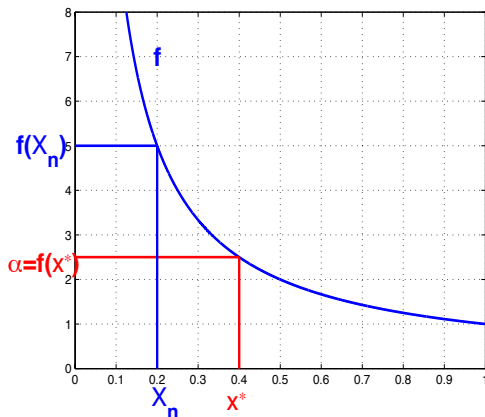
Stochastic approximation for $d = 1$.



Goal

→ Find the value x^* with very few knowledge on f .

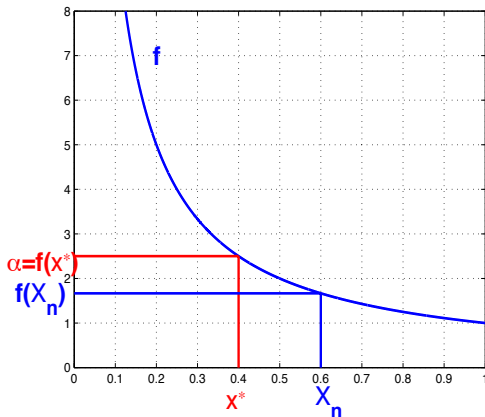
Stochastic approximation.



Basic Idea

If you are able to say that $f(X_n) > \alpha$, then increase the value of X_n .

Stochastic approximation.



Basic Idea

If you are able to say that $f(X_n) < \alpha$, then decrease the value of X_n .

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The Robbins-Monro algorithm.

Let (γ_n) be a sequence of positive real numbers decreasing to zero

$$\sum_{n=1}^{\infty} \gamma_n = +\infty \quad \text{and} \quad \sum_{n=1}^{\infty} \gamma_n^2 < +\infty.$$

For the sake of simplicity, we shall make use of

$$\gamma_n = \frac{1}{n}.$$

The Robbins-Monro algorithm

$$\mathbf{X}_{n+1} = \mathbf{X}_n + \gamma_n (\mathbf{Y}_{n+1} - \alpha)$$

where the initial state X_0 is a square integrable random vector of \mathbb{R}^d which can be arbitrarily chosen.

Almost sure convergence.

Let g be the positive function defined on \mathbb{R}^d by

$$g(X_n) = \mathbb{E}[\|Y_{n+1}\|^2 | \mathcal{F}_n].$$

Theorem (Robbins-Monro)

Assume that the function f is continuous from \mathbb{R}^d to \mathbb{R}^d such that $f(x^*) = \alpha$, and for all x different from x^* ,

$$\langle x - x^*, f(x) - \alpha \rangle < 0.$$

Assume that for $K > 0$ and for all $x \in \mathbb{R}^d$,

$$g(x) \leq K(1 + \|x\|^2).$$

Then, we have the almost sure convergence

$$\lim_{n \rightarrow \infty} X_n = x^* \quad \text{a.s.}$$

Proof of the almost sure convergence.

Proof.

First of all, denote

$$V_n = \|X_n - x^*\|^2.$$

For all $n \geq 0$, we clearly have

$$\begin{aligned} V_{n+1} &= \|X_{n+1} - x^*\|^2, \\ &= \|X_n + \gamma_n(Y_{n+1} - \alpha) - x^*\|^2, \\ &= \|X_n - x^*\|^2 + 2\gamma_n \langle X_n - x^*, Y_{n+1} - \alpha \rangle + \gamma_n^2 \|Y_{n+1} - \alpha\|^2, \end{aligned}$$

which leads to

$$V_{n+1} = V_n + \gamma_n^2 \|Y_{n+1} - \alpha\|^2 + 2\gamma_n \langle X_n - x^*, f(X_n) + \varepsilon_{n+1} - \alpha \rangle$$

where $\varepsilon_{n+1} = Y_{n+1} - f(X_n)$. □

Proof of the almost sure convergence, continued

Proof.

Since $\mathbb{E}[Y_{n+1}|\mathcal{F}_n] = f(X_n)$, $\mathbb{E}[\varepsilon_{n+1}|\mathcal{F}_n] = 0$. It means that (ε_n) is a **martingale difference sequence**. Consequently,

$$\mathbb{E}[V_{n+1}|\mathcal{F}_n] = V_n + \gamma_n^2 \mathbb{E}[\|Y_{n+1} - \alpha\|^2|\mathcal{F}_n] - B_n$$

where (B_n) is the positive sequence given by

$$B_n = -2\gamma_n \langle X_n - x^*, f(X_n) - \alpha \rangle$$

Moreover,

$$\mathbb{E}[\|Y_{n+1}\|^2|\mathcal{F}_n] \leq K(1 + \|X_n\|^2) \leq L(1 + V_n)$$

where $L = 2K(1 + \|x^*\|^2)$. □

Proof of the almost sure convergence, continued

Proof.

Therefore, we obtain that

$$\mathbb{E}[V_{n+1} | \mathcal{F}_n] \leq V_n(1 + a_n) + A_n - B_n$$

where $a_n = 2L\gamma_n^2$ and $A_n = 2(L + \|\alpha\|^2)\gamma_n^2$. The assumption

$$\sum_{n=1}^{\infty} \gamma_n^2 < +\infty$$

clearly implies that

$$\sum_{n=1}^{\infty} a_n < +\infty \quad \text{and} \quad \sum_{n=1}^{\infty} A_n < +\infty \quad \text{a.s.}$$



Proof of the almost sure convergence, continued

Proof.

Hence, it follows from Robbins-Siegmund theorem that (V_n) converges a.s. to a random variable V_∞ and

$$\sum_{n=1}^{\infty} B_n < +\infty \quad \text{a.s.}$$

It remains to prove that $V_\infty = 0$. Assume by contradiction that $V_\infty > 0$. Then, we can find two finite constants $0 < a < b$ such that, for n large enough, $a \leq \|X_n - x^*\| \leq b$. Denote by Δ the annulus of \mathbb{R}^d ,

$$\Delta = \left\{ x \in \mathbb{R}^d \text{ such that } a \leq \|x - x^*\| \leq b \right\}.$$

Let F be the continuous negative function defined, for all $x \in \mathbb{R}^d$, by

$$F(x) = \langle x - x^*, f(x) - \alpha \rangle.$$

Proof.

One can find $c > 0$ such that, for all $x \in \Delta$,

$$F(x) \leq -c.$$

However, for n large enough $X_n \in \Delta$, which implies that $F(X_n) \leq -c$.
Consequently, for n large enough,

$$B_n = -2\gamma_n F(X_n) \geq 2c\gamma_n.$$

Finally, the assumption

$$\sum_{n=1}^{\infty} \gamma_n = +\infty \quad \implies \quad \sum_{n=1}^{\infty} B_n = +\infty$$

leading to a contradiction. It means that $V_{\infty} = 0$ so $X_n \rightarrow x^*$ a.s.



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Asymptotic normality.

The asymptotic normality requires more assumption on the function f . We now assume that f is twice differentiable. It follows from **Taylor's formula** that

$$f(x) = \alpha + H(x - x^*) + O(\|x - x^*\|^2)$$

where H is the **Jacobian matrix** of f at x^* . We also assume that H is an **Hurwitz matrix**. It means that the real parts of all the eigenvalues of H are negative. Let $\lambda_{\max}(H)$ be the eigenvalue of H with the largest real part and denote

$$\rho = -\operatorname{Re}(\lambda_{\max}(H)).$$

In dimension $d = 1$, we have $f(x^*) = \alpha$, $H = f'(x^*)$ and $\rho = -f'(x^*)$.

Asymptotic normality, continued.

Let (ε_n) be the **martingale difference sequence** given by

$$\varepsilon_{n+1} = Y_{n+1} - \mathbb{E}[Y_{n+1}|\mathcal{F}_n] = Y_{n+1} - f(X_n).$$

Theorem (Robbins-Monro, continued)

Assume that the function f is twice differentiable from \mathbb{R}^d to \mathbb{R}^d such that $f(x^) = \alpha$. Suppose that f and g satisfy the same assumptions as in Robbins-Monro Theorem. Moreover, assume that*

$$\lim_{n \rightarrow \infty} \mathbb{E}[\varepsilon_{n+1} \varepsilon_{n+1}^T | \mathcal{F}_n] = \Gamma \quad \text{a.s.}$$

where Γ is a symmetric definite positive matrix and that (ε_n) has a conditional moment of order > 2 . If $\rho > 1/2$, we have the asymptotic normality

$$\sqrt{n}(\mathbf{X}_n - \mathbf{x}^*) \xrightarrow{\mathcal{L}} \mathcal{N}(\mathbf{0}, \Sigma).$$

Asymptotic normality for $d = 1$.

The limiting covariance matrix Σ is the unique solution of the **Lyapunov equation**

$$\left(H + \frac{1}{2}I_d\right)\Sigma + \Sigma\left(H^T + \frac{1}{2}I_d\right) = -\Gamma.$$

It is quite complicated to evaluate Σ . However, in the special case $d = 1$ and $\Gamma = \sigma^2$, we have $\rho = -H = -f'(x^*)$,

$$\Sigma = \frac{\sigma^2}{2\rho - 1}.$$

Consequently, as soon as $\rho > 1/2$, we have

$$\sqrt{n}(\mathbf{X}_n - \mathbf{x}^*) \xrightarrow{\mathcal{L}} \mathcal{N}\left(\mathbf{0}, \frac{\sigma^2}{2\rho - 1}\right).$$

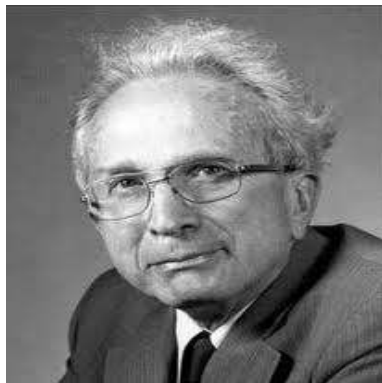
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Stochastic approximation.



Jack Kiefer



Jacob Wolfowitz

Stochastic approximation.

Let f be an **unknown differentiable function** from \mathbb{R}^d to \mathbb{R} .

Goal

→ Find a vector \mathbf{x}^* of \mathbb{R}^d which satisfies

$$\nabla f(\mathbf{x}^*) = \mathbf{0}.$$

We will make use of the **directional derivative** of f at $\mathbf{x} \in \mathbb{R}^d$ along the vector $\mathbf{y} \in \mathbb{R}^d$, given by

$$\langle \nabla f(\mathbf{x}), \mathbf{y} \rangle = \lim_{t \rightarrow 0} \frac{f(\mathbf{x} + t\mathbf{y}) - f(\mathbf{x} - t\mathbf{y})}{2t}.$$

Stochastic approximation.

We will assume in all the sequel that for all $n \geq 1$, we can compute X_1, \dots, X_n of \mathbb{R}^d and we can find Y_{n+1} and Z_{n+1} of \mathbb{R}^d such that

$$\mathbb{E}[Y_{n+1} | \mathcal{F}_n] = \begin{pmatrix} f(X_n + c_n e_1) \\ \vdots \\ f(X_n + c_n e_d) \end{pmatrix} = \Phi(X_n)$$

and

$$\mathbb{E}[Z_{n+1} | \mathcal{F}_n] = \begin{pmatrix} f(X_n - c_n e_1) \\ \vdots \\ f(X_n - c_n e_d) \end{pmatrix} = \Psi(X_n)$$

where (e_1, \dots, e_d) is the canonical basis of \mathbb{R}^d , (c_n) is a sequence of positive real numbers decreasing to zero, and $\mathcal{F}_n = \sigma(X_1, \dots, X_n)$. In dimension $d = 1$, $\mathbb{E}[Y_{n+1} | \mathcal{F}_n] = f(X_n + c_n)$, $\mathbb{E}[Z_{n+1} | \mathcal{F}_n] = f(X_n - c_n)$.

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The Kiefer-Wolfowitz algorithm.

Let (γ_n) be a sequence of positive real numbers decreasing to zero

$$\sum_{n=1}^{\infty} \gamma_n = +\infty, \quad \sum_{n=1}^{\infty} \left(\frac{\gamma_n}{c_n}\right)^2 < +\infty, \quad \sum_{n=1}^{\infty} \gamma_n c_n < +\infty.$$

For the sake of simplicity, we can choose $0 < c < 1/2$,

$$\gamma_n = \frac{1}{n} \quad \text{and} \quad c_n = \frac{1}{n^c}.$$

The Kiefer-Wolfowitz algorithm

$$X_{n+1} = X_n + \frac{\gamma_n}{2c_n} (Y_{n+1} - Z_{n+1})$$

where the initial state X_0 is a square integrable random vector of \mathbb{R}^d which can be arbitrarily chosen.

Almost sure convergence.

Let g and h be the two positive functions defined on \mathbb{R}^d by

$$g(X_n) = \mathbb{E}[\|Y_{n+1}\|^2 | \mathcal{F}_n] \quad \text{and} \quad h(X_n) = \mathbb{E}[\|Z_{n+1}\|^2 | \mathcal{F}_n].$$

Theorem (Kiefer-Wolfowitz)

Assume that the function f is twice continuously differentiable from \mathbb{R}^d to \mathbb{R} such that $\nabla f(x^) = 0$, and for all x different from x^* ,*

$$\langle x - x^*, \nabla f(x) \rangle < 0.$$

Assume that for $L > 0$ and for all $x \in \mathbb{R}^d$,

$$\|\nabla^2 f(x)\| \leq L(1 + \|x\|).$$

Almost sure convergence, continued

Theorem (Kiefer-Wolfowitz, continued)

Moreover, assume that for $K_g > 0$, $K_h > 0$ and for all $x \in \mathbb{R}^d$,

$$g(x) \leq K_g(1 + \|x\|^2) \quad \text{and} \quad h(x) \leq K_h(1 + \|x\|^2).$$

Then, we have the almost sure convergence

$$\lim_{n \rightarrow \infty} X_n = x^* \quad \text{a.s.}$$

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Asymptotic normality.

The asymptotic normality requires more assumption on the function f . We now assume that $f \in \mathcal{C}^3(\mathbb{R}^d)$ with $\nabla f(x^*) = 0$. As $\nabla f \in \mathcal{C}^2(\mathbb{R}^d)$, it follows from **Taylor's formula** that

$$\nabla f(x) = H(x - x^*) + O(\|x - x^*\|^2)$$

where $H = \nabla^2 f(x^*)$ is the **Hessian matrix** of f at x^* . We also assume that H is a **negative definite matrix**. It means that all the eigenvalues of H are negative. Denote

$$\rho = -\lambda_{\max}(H).$$

In dimension $d = 1$, we have $f'(x^*) = 0$, $H = f''(x^*)$ and $\rho = -f''(x^*)$.

Asymptotic normality, continued

Let (ε_n) and (ξ_n) be the **martingale difference sequences** given by

$$\varepsilon_{n+1} = Y_{n+1} - \mathbb{E}[Y_{n+1}|\mathcal{F}_n] = Y_{n+1} - \Phi(X_n),$$

$$\xi_{n+1} = Z_{n+1} - \mathbb{E}[Z_{n+1}|\mathcal{F}_n] = Z_{n+1} - \Psi(X_n).$$

Theorem (Kiefer-Wolfowitz, continued)

Assume that the function $f \in \mathcal{C}^3(\mathbb{R}^d)$ such that $\nabla f(x^*) = 0$. Suppose that f and g satisfy the same assumptions as in Kiefer-Wolfowitz Theorem. Moreover, assume that

$$\lim_{n \rightarrow \infty} \mathbb{E}[\varepsilon_{n+1} \varepsilon_{n+1}^T | \mathcal{F}_n] = \Gamma_g \quad \text{a.s.}$$

$$\lim_{n \rightarrow \infty} \mathbb{E}[\xi_{n+1} \xi_{n+1}^T | \mathcal{F}_n] = \Gamma_h \quad \text{a.s.}$$

where Γ_g and Γ_h are symmetric definite positive matrices and that (ε_n) and (ξ_n) have conditional moments of order **> 2**.

Asymptotic normality, continued

Theorem (Kiefer-Wolfowitz, continued)

If $\rho > 2c$ where $1/6 < c < 1/2$, we have the asymptotic normality

$$\sqrt{nc_n^2}(\mathbf{X}_n - \mathbf{x}^*) \xrightarrow{\mathcal{L}} \mathcal{N}(\mathbf{0}, \Sigma).$$

→ In the special case $\rho > 2c$ with $c = 1/6$, we also have

$$n^{1/3}(\mathbf{X}_n - \mathbf{x}^*) \xrightarrow{\mathcal{L}} \mathcal{N}(m, \Sigma)$$

where the mean m can be explicitly calculated.

Asymptotic normality for $d = 1$.

The limiting covariance matrix Σ is the unique solution of the **Lyapunov equation**

$$\left(H + \left(\frac{1}{2} - c\right)I_d\right)\Sigma + \Sigma\left(H + \left(\frac{1}{2} - c\right)I_d\right) = -\frac{1}{4}\Gamma.$$

It is quite complicated to evaluate Σ . However, in the special case $d = 1$ and $\Gamma = \sigma^2$, we have

$$\Sigma = \frac{\sigma^2}{8(\rho + c - 1/2)}.$$

Consequently, as soon as $\rho > 2c$ where $1/6 < c < 1/2$, we have

$$\sqrt{nc_n^2}(\mathbf{X}_n - \mathbf{x}^*) \xrightarrow{\mathcal{L}} \mathcal{N}\left(\mathbf{0}, \frac{\sigma^2}{8(\rho + c - 1/2)}\right).$$

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Stochastic averaging.



David Ruppert



Boris Polyak

Stochastic averaging.

The idea of using averaging to accelerate stochastic algorithms is due to Polyak and Ruppert. It consists in introducing a Cesaro mean over the iterations of the original stochastic algorithm

$$\bar{X}_n = \frac{1}{n} \sum_{k=1}^n X_k.$$

Goal

- Improve the convergence properties of the stochastic algorithm by minimizing its asymptotic variance.
- Substantially weaken the conditions of the previous asymptotic results on the stochastic algorithm.

Stochastic averaging on the Robbins-Monro algorithm.

Consider the slow down Robbins-Monro algorithm given by

$$\mathbf{X}_{n+1} = \mathbf{X}_n + \gamma_n (\mathbf{Y}_{n+1} - \alpha)$$

where the initial state X_0 is a square integrable random vector of \mathbb{R}^d which can be arbitrarily chosen and the step

$$\gamma_n = \frac{1}{n^c} \quad \text{with} \quad \frac{1}{2} < c < 1.$$

At time $n \geq 1$, compute de Cesaro mean

$$\bar{\mathbf{X}}_n = \frac{1}{n} \sum_{k=1}^n \mathbf{X}_k.$$

A second-order recursive equation.

We have

$$(n+1)\bar{X}_{n+1} = \sum_{k=1}^n X_k + X_{n+1} = n\bar{X}_n + X_{n+1},$$

which implies that

$$\bar{X}_{n+1} = \bar{X}_n + \frac{1}{n+1} (X_{n+1} - \bar{X}_n).$$

However,

$$X_{n+1} = X_n + \gamma_n (Y_{n+1} - \alpha).$$

A second-order recursive equation.

Consequently, as $X_n = n\bar{X}_n - (n-1)\bar{X}_{n-1}$ we obtain that

$$\begin{aligned}\bar{X}_{n+1} &= \bar{X}_n + \frac{1}{n+1} \left(X_n - \bar{X}_n + \gamma_n (Y_{n+1} - \alpha) \right), \\ &= \bar{X}_n + \frac{1}{n+1} \left((n-1)(\bar{X}_n - \bar{X}_{n-1}) + \gamma_n (Y_{n+1} - \alpha) \right), \\ &= \bar{X}_n + \left(\frac{n-1}{n+1} \right) \bar{X}_n - \left(\frac{n-1}{n+1} \right) \bar{X}_{n-1} + \frac{\gamma_n}{n+1} (Y_{n+1} - \alpha),\end{aligned}$$

leading to **the second-order recursive equation**

$$\bar{X}_{n+1} = \left(\frac{2n}{n+1} \right) \bar{X}_n - \left(\frac{n-1}{n+1} \right) \bar{X}_{n-1} + \frac{\gamma_n}{n+1} (Y_{n+1} - \alpha).$$

A second-order recursive equation.

Consequently, as $X_n = n\bar{X}_n - (n-1)\bar{X}_{n-1}$ we obtain that

$$\begin{aligned}\bar{X}_{n+1} &= \bar{X}_n + \frac{1}{n+1} \left(X_n - \bar{X}_n + \gamma_n (Y_{n+1} - \alpha) \right), \\ &= \bar{X}_n + \frac{1}{n+1} \left((n-1)(\bar{X}_n - \bar{X}_{n-1}) + \gamma_n (Y_{n+1} - \alpha) \right), \\ &= \bar{X}_n + \left(\frac{n-1}{n+1} \right) \bar{X}_n - \left(\frac{n-1}{n+1} \right) \bar{X}_{n-1} + \frac{\gamma_n}{n+1} (Y_{n+1} - \alpha),\end{aligned}$$

leading to **the second-order recursive equation**

$$\bar{X}_{n+1} = \left(\frac{2n}{n+1} \right) \bar{X}_n - \left(\frac{n-1}{n+1} \right) \bar{X}_{n-1} + \frac{\gamma_n}{n+1} (Y_{n+1} - \alpha).$$

A second-order recursive equation.

Consequently, as $X_n = n\bar{X}_n - (n-1)\bar{X}_{n-1}$ we obtain that

$$\begin{aligned}\bar{X}_{n+1} &= \bar{X}_n + \frac{1}{n+1} \left(X_n - \bar{X}_n + \gamma_n (Y_{n+1} - \alpha) \right), \\ &= \bar{X}_n + \frac{1}{n+1} \left((n-1) (\bar{X}_n - \bar{X}_{n-1}) + \gamma_n (Y_{n+1} - \alpha) \right), \\ &= \bar{X}_n + \left(\frac{n-1}{n+1} \right) \bar{X}_n - \left(\frac{n-1}{n+1} \right) \bar{X}_{n-1} + \frac{\gamma_n}{n+1} (Y_{n+1} - \alpha),\end{aligned}$$

leading to **the second-order recursive equation**

$$\bar{X}_{n+1} = \left(\frac{2n}{n+1} \right) \bar{X}_n - \left(\frac{n-1}{n+1} \right) \bar{X}_{n-1} + \frac{\gamma_n}{n+1} (Y_{n+1} - \alpha).$$

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Almost sure convergence.

Theorem (Robbins-Monro averaging)

Assume that the function f is continuous from \mathbb{R}^d to \mathbb{R}^d such that $f(x^*) = \alpha$, and for all x different from x^* ,

$$\langle x - x^*, f(x) - \alpha \rangle < 0.$$

Assume that for $K > 0$ and for all $x \in \mathbb{R}^d$,

$$g(x) \leq K(1 + \|x\|^2).$$

Then, we have the almost sure convergence

$$\lim_{n \rightarrow \infty} \bar{X}_n = x^* \quad \text{a.s.}$$

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Asymptotic normality.

Theorem (Robbins-Monro averaging)

Assume that the function f is twice differentiable from \mathbb{R}^d to \mathbb{R}^d such that $f(x^*) = \alpha$. Suppose that f and g satisfy the same assumptions as in Robbins-Monro Theorem. Moreover, assume that

$$\lim_{n \rightarrow \infty} \mathbb{E}[\varepsilon_{n+1} \varepsilon_{n+1}^T | \mathcal{F}_n] = \Gamma \quad \text{a.s.}$$

where Γ is a symmetric definite positive matrix and that (ε_n) has a conditional moment of order > 2 . Then, we have the asymptotic normality

$$\sqrt{n}(\bar{X}_n - x^*) \xrightarrow{\mathcal{L}} \mathcal{N}(0, \Sigma)$$

where the asymptotic matrix Σ is given by

$$\Sigma = H^{-1} \Gamma (H^{-1})^T.$$

Asymptotic normality for $d = 1$.

It is not necessary to assume that

$$\rho = -\operatorname{Re}(\lambda_{\max}(\mathbf{H})) > \frac{1}{2}.$$

In the special case $d = 1$ and $\Gamma = \sigma^2$, we have $\rho = -H = -f'(x^*)$, which means that

$$\Sigma = \frac{\sigma^2}{(f'(x^*))^2}.$$

Consequently, the asymptotic normality reduces to

$$\sqrt{n}(\bar{\mathbf{X}}_n - \mathbf{x}^*) \xrightarrow{\mathcal{L}} \mathcal{N}\left(\mathbf{0}, \frac{\sigma^2}{(f'(x^*))^2}\right).$$

