ON THE OPTIMALITY OF THE MONTE-CARLO ESTIMATOR

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Abstract. We prove that on an atomless probability space, the worst-case mean squared error of the Monte-Carlo estimator is minimal if the random points are chosen independently.

1. Introduction and statement of the results

Let \((X, \mu)\) be a probability space. We are interested in the following general question: if \(f\) is a measurable, real or complex-valued function on \(X\), how can we efficiently compute the integral \(\int_X f \, d\mu\)? The famous Monte-Carlo method is a solution to this problem: just choose an integer \(n\) big enough, and draw \(Z_1, \ldots, Z_n\) independent \(X\)-valued random variables (that is, random points) of law \(\mu\), and form the mean \(\frac{1}{n} \sum_{i=1}^{n} f(Z_i)\), called the Monte-Carlo estimator.

We measure the quality of this method by computing what we call the mean squared error:

\[
\text{Var} \left( \frac{1}{n} \sum_{i=1}^{n} f(Z_i) - \int_X f \, d\mu \right) = \frac{1}{n} \left\| f - \int_X f \, d\mu \right\|_{L^2(X, \mu)}^2
\]

and we obtain the following equality, concerning the worst-case mean squared error:

\[
\sup_{f \in L^2(X, \mu)} \text{Var} \left( \frac{1}{n} \sum_{i=1}^{n} f(Z_i) - \int_X f \, d\mu \right) = \frac{1}{n}.
\]

In this paper, we study the question of measuring the worst-case mean squared error, in the general situation where the points \(Z_i\) are not supposed independent, and we prove the following theorem and its corollary.

**Theorem.** Let \((X, \mu)\) be a probability space, let \(N, n \in \mathbb{N}^*\), and \(Z := (Z_1, \ldots, Z_n)\) an \(n\)-tuple of random points on \(X\) such that for all \(i\), the law of \(Z_i\) is \(\mu\). We do not assume that the \(Z_i\)'s are independent. Furthermore, we assume that \(X\) can be partitioned in \(N\) measurable subsets of equal measure.

We then have

\[
\sup_{f \in L^2(X, \mu), \, \|f\|_2 = 1} \text{Var} \left( \frac{1}{n} \sum_{i=1}^{n} f(Z_i) - \int_X f \, d\mu \right) \geq \frac{1}{n} \left( 1 - \frac{n-1}{N-1} \right).
\]

**Corollary.** Let \((X, \mu)\) be an atomless probability space, \(n \in \mathbb{N}^*\), and \(Z := (Z_1, \ldots, Z_n)\) an \(n\)-tuple of random points on \(X\) such that for all \(i\), the law of \(Z_i\) is \(\mu\). We do not assume that the \(Z_i\)'s are independent.

We then have

\[
\sup_{f \in L^2(X, \mu), \, \|f\|_2 = 1} \text{Var} \left( \frac{1}{n} \sum_{i=1}^{n} f(Z_i) - \int_X f \, d\mu \right) \geq \frac{1}{n}.
\]

**Remark.** As we shall see in the paper, in the case where \(X := \{1, \ldots, N\}\) and \(\mu\) is the uniform measure on \(X\), the inequality of the theorem is an equality when the law of \(Z\) is the uniform measure on the set of \(n\)-tuples of points in \(X\) such that the coordinates are pairwise different. This random \(n\)-tuple is then, in the sense of the worst-case mean squared error, than an independent \(n\)-tuple.
As we saw before, the inequality in the corollary is an equality if the $Z_i$’s are independent. We don’t know if this condition is necessary. It is, to our opinion, worth knowing that in [LPS86], the authors build, for all prime $p$ such that $p \equiv 1[4]$, a $(p+1)$-tuple $Z$ of uniform random points on the 2-sphere which are not independent, and prove that its worst-case mean squared error is $\frac{4p}{p+1}$, which is approximately 4 times the lower bound in the corollary. In the article [LP18], it is shown that their construction is optimal, in a broad framework.

We confess our astonishment of having found no trace of these statements, which answer a question that we find both natural and general, and in an elementary way.

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2. Proofs

To alleviate the presentation, we use the following notation: we consider the numbers

$$\operatorname{MSE}_Z(f) := \operatorname{Var} \left( \frac{1}{n} \sum_{i=1}^{n} f(Z_i) - \int_X f \, d\mu \right)$$

et

$$\operatorname{MSE}(Z) := \sup_{f \in L^2(X,\mu)} \operatorname{MSE}_Z(f).$$

First of all, if $f \in L^2(X,\mu)$, we notice that $\operatorname{MSE}_Z(f) = \operatorname{MSE}(Z) \left( f - \int_X f \, d\mu \right)$. Consequently, $\operatorname{MSE}(Z)$ is also the sup of the $\operatorname{MSE}_Z(f)$ for $f$ of norm 1 zero integral.

Let $f \in L^2(X,\mu)$, of norm 1 and zero integral. We have that

$$\operatorname{MSE}_Z(f) = \mathbb{E} \left[ \left( \frac{1}{n} \sum_{i=1}^{n} f(Z_i) \right)^2 \right]$$

$$= \mathbb{E} \left[ \frac{1}{n^2} \sum_{i=1}^{n} f(Z_i)^2 + \frac{1}{n^2} \sum_{i \neq j} f(Z_i) f(Z_j) \right]$$

$$= \frac{1}{n^2} \sum_{i=1}^{n} \mathbb{E}[f(Z_i)^2] + \frac{1}{n^2} \sum_{i \neq j} \mathbb{E}[f(Z_i) f(Z_j)]$$

$$= \frac{1}{n} + \frac{1}{n^2} \sum_{i \neq j} \mathbb{E}[f(Z_i) f(Z_j)]$$

and we recover the fact recalled above: if the $Z_i$’s are pairwise independent, and if $f$ is of norm 1 of zero integral, $\operatorname{MSE}_Z(f) = \frac{1}{n}$.

Let us prove the theorem.

Proof of the theorem. Let $X_1, \ldots, X_N$ be measurable subsets that partition $X$, all of measure $\frac{1}{N}$, with $N \geq 2$. Let us denote, for $p \in \{1, \ldots, N\}$, $\mu_p := \mu(X_p)$. For every $(p,q) \in \{1, \ldots, N\}^2$, we set

$$f_{p,q} := \sqrt{\frac{N}{2}} 1_{X_p} - \sqrt{\frac{N}{2}} 1_{X_q}.$$

Moreover, we will denote, for $k \in \{1, \ldots, N\}$, $f_{p,q}(X_k)$ the value that $f_{p,q}$ takes on $X_k$ - this abuse of notation is harmless because $f_{p,q}$ is constant on the $X_i$’s.

$f_{p,q}$ is visibly of zero integral, and if $p \neq q$, its norm is 1.

We will prove that there are different $p,q \in \{1, \ldots, N\}$ such that $\operatorname{MSE}_Z(f_{p,q}) \geq \frac{1}{n} \left( 1 - \frac{n-1}{N-1} \right)$. 

Let \( p, q \in \{1, \ldots, N\} \). We have that
\[
\text{MSE}_Z(f_{p,q}) = \frac{1}{n} + \frac{1}{n^2 \sum_{i\neq j}} \mathbb{E}\left[f_{p,q}(Z_i)f_{p,q}(Z_j)\right]
\]
\[
= \frac{1}{n} + \frac{1}{n^2 \sum_{i\neq j}} \left( \sum_k \mathbb{P}(Z_i \in X_k \text{ et } Z_j \in X_k) f_{p,q}(X_k)^2 \right)
\]
\[
\quad + \sum_{l \neq m} \mathbb{P}(Z_i \in X_l \text{ et } Z_j \in X_m) f_{p,q}(X_l) f_{p,q}(X_m)
\]
\[
= \frac{1}{n} + \frac{1}{n^2} \sum_{i \neq j} \left( \mathbb{P}(Z_i \in X_p \text{ et } Z_j \in X_p) \right)
\]
\[
+ \mathbb{P}(Z_i \in X_q \text{ et } Z_j \in X_q) - \mathbb{P}(Z_i \in X_p \text{ et } Z_j \in X_q)
\]
\[
- \mathbb{P}(Z_i \in X_q \text{ et } Z_j \in X_p) .
\]

from which we deduce the inequality
\[
\text{MSE}_Z(f_{p,q}) \geq \frac{1}{n} - \frac{1}{n^2} \frac{N}{2} \left( \sum_{i \neq j} \mathbb{P}(Z_i \in X_p \text{ et } Z_j \in X_q) + \mathbb{P}(Z_i \in X_q \text{ et } Z_j \in X_p) \right).
\]

Let us denote
\[\theta_{p,q} := \sum_{i \neq j} \mathbb{P}(Z_i \in X_p \text{ et } Z_j \in X_q) + \mathbb{P}(Z_i \in X_q \text{ et } Z_j \in X_p).\]

Let us compute:
\[
\sum_{p \neq q} \theta_{p,q} = 2 \sum_{p \neq q} \sum_{i \neq j} \mathbb{P}(Z_i \in X_p \text{ et } Z_j \in X_q)
\]
\[
= 2 \sum_{i \neq j} \sum_{p \neq q} \mathbb{P}(Z_i \in X_p \text{ et } Z_j \in X_q)
\]
\[
= 2 \sum_{i \neq j} \mathbb{P}(Z_i \text{ et } Z_j \text{ ne sont pas dans le même morceau de la partition})
\]
\[
\leq 2n(n-1).
\]

Now, since this sum of \( N(N-1) \) numbers is lower or equal than \( 2n(n-1) \), then one of the terms must be lower or equal than \( 2 \frac{n(n-1)}{N(N-1)} \). For a couple \((p,q)\) such that \( \theta_{p,q} \leq 2 \frac{n(n-1)}{N(N-1)} \), we then have
\[
\text{MSE}_Z(f_{p,q}) \geq \frac{1}{n} - \frac{1}{n^2} \frac{n(N-1)}{2} \frac{n(n-1)}{N(N-1)}
\]
\[
= \frac{1}{n} - \frac{n}{n(N-1)}
\]
\[
= \frac{1}{n} \left(1 - \frac{n-1}{N-1}\right).
\]

Here’s an example where the inequality is an equality.

**Proposition.** If \( X := \{1, \ldots, N\} \), if \( \mu \) is the uniform probability on \( X \), if \( n \leq N \), and if the law of \( Z \) is the uniform measure on the set of \( n \)-tuples of points in \( X \) which coordinates are pairwise different, then the inequality in the theorem is an equality, that is,
\[
\text{MSE}_Z = \frac{1}{n} \left(1 - \frac{n-1}{N-1}\right).
\]

**Proof.** Let \( \pi \) be the measure on \( X^n \) defined by
\[
\pi := \frac{(N-n)!}{N!} \sum_{\delta(i_1, \ldots, i_n)} \delta(i_1, \ldots, i_n),
\]

where \( \delta \) is the Kronecker delta function.
where $\delta$ is the notation for a Dirac measure. In words, $\pi$ is the uniform measure on the set of $n$-tuples of points in $X$ which coordinates are pairwise different. Let $Z = (Z_1, \cdots, Z_n)$ be an $n$-tuple of law $\pi$ (we then have, for all $i$, that $Z_i$ is uniform on $X$).

Let $f \in L^2(X, \mu)$ be of norm $1$, and such that $\int f \, d\mu = 0$. Let us compute:

$$
\sum_{l \neq m} \mathbb{E}[f(Z_l)f(Z_m)] = \sum_{l \neq m} \mathbb{E} \left[ \sum_{A \subseteq X} \sum_{|A|=n, i_j \neq k} 1_{\{Z_1 = i_1, \cdots, Z_n = i_n\}} f(Z_l)f(Z_m) \right]
$$

$$
= \sum_{l \neq m} \sum_{A \subseteq X} \sum_{|A|=n, i_j \neq k} \mathbb{P}[Z_1 = i_1, \cdots, Z_n = i_n] f(i_l)f(i_m)
$$

$$
= \binom{N}{n}^{-1} \sum_{A \subseteq X} \sum_{|A|=n, p \neq q} f(p)f(q)
$$

$$
= \frac{(N-2)}{n-2} \binom{N}{n}^{-1} \sum_{p \neq q} f(p)f(q)
$$

$$
= \frac{n(n-1)}{N(N-1)} \sum_{p \in X} f(p) \sum_{q \in X, q \neq p} f(q)
$$

$$
= \frac{n(n-1)}{n(n-1)} \frac{\|f\|_2^2}{N-1}
$$

We therefore have

$$
\text{MSE}_Z(f) = \frac{1}{n} \left( 1 - \frac{n-1}{N-1} \right).
$$

Let us prove the corollary.

**Proof of the corollary.** We will prove that for all $\epsilon > 0$, we have that $\text{MSE}(Z) \geq \frac{1}{n} - \epsilon$, which is enough. According to a theorem of Sierpiński [Sie22], every atomless probability space is such that for every $a \in [0, 1]$, there is a measurable subset of $X$ of measure $a$. From this, it is easy, for all arbitrarily big $N$, to partition $X$ in $N$ of measurable subsets of equal measure. If we choose $N$ such that $\frac{1}{n} \left( 1 - \frac{n-1}{N-1} \right) \geq \frac{1}{n} - \epsilon$, which is obviously possible, then according to the theorem, it is possible to find $f$ of norm $1$, zero integral, such that $\text{MSE}_Z(f) \geq \frac{1}{n} - \epsilon$. □

For the sake of completeness, we add a simple proof of Sierpiński’s theorem.

**Complement** (Sierpiński’s theorem on atomless probability spaces). *If $(X, \mathcal{B}, \mu)$ is an atomless probability space, then for every measurable $A \subseteq X$, there exists $\phi : [0, \mu(A)] \to \mathcal{B}$ non-decreasing, such that $\forall t \in [0, \mu(A)], \quad \mu(\phi(t)) = t$.*

**Proof.** The hypothesis of $X$ being atomless means that for every measurable $B \subseteq X$ such that $\mu(B) > 0$, there exists a measurable $C \subseteq B$ such that $0 < \mu(C) < \mu(B)$.

Let $A$ be a measurable subset of $X$, such that $\mu(A) > 0$ (if $\mu(A) = 0$, it is enough to define $\phi(0) := A$). By applying Zorn’s lemma, we obtain a $\phi : I \to \mathcal{B}$ where $I$ is a subset of $[0, \mu(A)]$, $\phi$ is non-decreasing, such that $\forall i \in I$, $\mu(\phi(i)) = i$, and such that $\phi$ has no strict extension that satisfies these properties. Let us show that $I$ equals $[0, \mu(A)]$.

On the one hand, $I$ is closed. Indeed, let $(x_n)_{n \in \mathbb{N}}$ be a sequence of elements in $I$ that converges to some $x$. Let us show that $x \in I$. We can assume, up to extracting a subsequence, that $(x_n)_n$ is monotonous. If $x \notin I$, let us define $\phi := I \cup \{x\} \to \mathcal{B}$ that extends $\phi$ by defining
\( \tilde{\phi}(x) := \bigcap_n \phi(x_n) \) if \( (x_n) \) is non-increasing, and \( \tilde{\phi}(x) := \bigcup_n \phi(x_n) \) if \( (x_n) \) non-decreasing. According to \( \mu \)'s continuity properties, \( \mu(\phi(x)) = \lim_n x_n = x \), and according to the monotony properties of \( \mu \), \( \tilde{\phi} \) is non-decreasing. \( \tilde{\phi} \) is therefore a strict extension of \( \phi \) that verifies the same properties. This is a contradiction. So \( x \in I \), and therefore, \( I \) is closed.

On the other hand, \( I \) verifies \( \forall a, b \in I, a < b \Rightarrow (\exists c \in I, a < c < b) \) (we say that \( I \) is order-dense). Indeed, if there are \( a, b \in I \) such that \( a < b \) and \( ]a, b[ \cap I = \emptyset \), then let us use the hypothesis that \( X \) is atomless, which provides a measurable \( C \subset \phi(b) \setminus \phi(a) \) such that \( 0 < \mu(C) < b - a \). Let us then define \( \tilde{\phi} : I \cup \{ a + \mu(C) \} \) that extends \( \phi \) by defining \( \tilde{\phi}(a + \mu(C)) := \phi(a) \cup C \). Then \( \mu(\tilde{\phi})(a + \mu(C)) = \mu(\phi(a) \cup C) = a + \mu(C) \). According to \( \mu \)'s monotony properties, \( \tilde{\phi} \) est non-decreasing. \( \tilde{\phi} \) is then a strict extension of \( \phi \) that verifies the same properties. This is a contradiction. Therefore, \( I \) is order-dense.

So \( I \) is closed and order-dense. Therefore, \( I = [0, \mu(A)] \).

\[ \square \]

References

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