Minimizing the variance in the estimation of the performance of a method for the fully-automatic design of robot swarms: a mathematical proof

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Minimizing the variance in the estimation of the performance of a method for the fully-automatic design of robot swarms: a mathematical proof

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This technical document provides a complete proof of a theorem originally presented in Ligot et al. [1]. This theorem proposes a sampling strategy that minimizes the variance in the estimation of the real-world performance of fully-automatic methods, which are meant to design control software for robot swarms to solve a class of missions. Ganguli [2] and Marcuse [3] studied a formally identical problem applied to different contexts, and they both reached similar conclusions as we do in this document. Birattari [4, 5] studied the sampling strategy that is to be adopted when one desires to minimize the variance of the expected performance of a design method when solving specific missions.

A sampling strategy for estimating the expected performance of a design method on a class of missions, given that a maximum number $N$ of executions can be performed, can be formally described by a triple $\langle n_m, n_d, n_x \rangle$, with $\bar{N} := n_m \cdot n_d \cdot n_x \leq N$. The expected performance is estimated on the basis of $n_m$ missions, $n_d$ design processes per mission (to generate $n_d$ instances of control software per mission), and $n_x$ executions of each of them. We can assume that the cost (in abstract terms: time and resources) of running a design process is negligible compared to the one of running robot experiments. We can also assume that sampling a mission from a class of instances is inexpensive and that a sample of arbitrary size can be obtained. We also assume that, before running a design process on a given mission, we do not have any prior information on how well the control software we can generate automatically will perform and on what will be the variance of the performance. It has to be noticed that any triple $\langle n_m, n_d, n_x \rangle$ yields an unbiased estimate of the expected performance. Yet, different triples might differ for what concerns the variance of the estimate they yield.

**Theorem 1** Under the assumptions made above, given that a maximum number $N$ of executions can be performed, the sampling strategy described by the triple $E = \langle n_m, n_d, n_x \rangle$, with $n_m = N$, $n_d = 1$, and $n_x = 1$, is the one that minimizes the variance of the estimate.

The variance of the estimator $\hat{\mu}$ associated with the sampling strategy $E$ is

$$
E \left[ (\hat{\mu}_E - \mu)^2 \right] = \frac{\sigma^2_{AM}}{n_m} + \frac{\sigma^2_{AD}}{n_m n_d} + \frac{\sigma^2_{WM}}{n_m n_d n_x},
$$

(1)

where $\sigma^2_{AM}$ is the across-mission variance and indicates how missions differ from one another, $\sigma^2_{AD}$ is the expected across-design variance and indicates how designs differ from one another within a same mission (averaged across all possible missions), and $\sigma^2_{WM}$ is the expected within-mission variance and indicates how scores differ from one another within a same mission (averaged across all possible missions). Formal definitions of these three variances are given in Section 1. Clearly, to minimize the variance of the estimator the denominators need to be chosen so as to be as large as possible. It is straightforward to conclude that this will happen when $n_m = N$, $n_d = n_x = 1$, as $n_m \cdot n_d \cdot n_x \leq N$, which also implies that $n_m \cdot n_d \leq N$.

The remainder of this document is dedicated to deriving Equation 1.
1 Definitions

A sampling strategy $\mathcal{E} = \langle n_m, n_d, n_x \rangle$ is a triplet of integers where $n_m$ denotes the number of missions, $n_d$ the number of designs per mission (resulting in $n_d$ instances of control software), and $n_x$ the number of executions on the robots of each instance of control software. The total number of executions on the robots is denoted by $N = n_m \cdot n_d \cdot n_x$.

The joint probability of having to solve mission $m$, producing the design $d$, and eventually observing the score $s$ is:

$$P(s, d, m) = P_S(s|d, m)P_D(d|m)P_M(m),$$

where $P_M(m)$ is the probability of having to solve mission $m$; $P_D(d|m)$ is the conditional probability of producing design $d$, having to solve mission $m$; and $P_S(s|d, m)$ is the conditional probability of observing score $s$, while performing design $d$ on mission $m$. The expected value of $s$ with respect to this joint probability is:

$$\mu := \int s \ dP_M(m) \ dP_D(d|m) \ dP_S(s|d, m).$$

The expected value of the score within mission $m$ and within design $d$ for mission $m$ are respectively:

$$\mu_m := \int s \ dP_D(d|m) \ dP_S(s|d, m) \quad \text{and} \quad \mu_{md} := \int s \ dP_S(s|d, m).$$

The variance within mission $m$ is:

$$\sigma_m^2 := \int (s - \mu_m)^2 \ dP_D(d|m) \ dP_S(s|d, m).$$

The expected within-mission variance provides information on how scores differ one from the other within a same mission (averaged across all possible missions); it is defined as:

$$\bar{\sigma}^2_{WM} := \int \sigma_m^2 \ dP_M(m) = \int (s - \mu_m)^2 \ dP_M(m) \ dP_D(d|m) \ dP_S(s|d, m).$$

The across-design variance within mission $m$ is:

$$\sigma^2_{AD,m} := \int (\mu_{md} - \mu_m)^2 \ dP_D(d|m).$$

The expected across-design variance provides information on how designs differ one from the other within a same mission (averaged across all possible missions); it is defined as:

$$\bar{\sigma}^2_{AD} := \int \sigma^2_{AD,m} \ dP_M(m) = \int (\mu_{md} - \mu_m)^2 \ dP_M(m) \ dP_D(d|m).$$

The across-mission variance provides information on how missions differ one from the other; it is defined as:

$$\sigma^2_{AM} := \int (\mu_m - \mu)^2 \ dP_M(m).$$

In the following, with the notation: $\int f(v_1, v_2, \ldots, v_L) \bigotimes_{l=1}^{L} dP(v_l)$, we denote the sequence of nested integrals $\int \cdots \int f(v_1, v_2, \ldots, v_L) dP(v_1) dP(v_2) \ldots dP(v_L)$. 

2
2 Proof

The goal of this proof is to show that given the following estimator

\[ \hat{\mu} = \frac{1}{N} \sum_{i=1}^{n_m} \sum_{j=1}^{n_d} \sum_{k=1}^{n_x} s_{ijk}, \]

where \( s_{ijk} \) is the score (or performance) observed in the execution \( x_{ijk} \) of the instance of control software issued from the design \( d_{ij} \) on the mission \( m_i \), the variance of \( \hat{\mu} \) is:

\[ E[ (\hat{\mu} - \mu)^2 ] = \frac{\sigma^2_{AM}}{n_m} + \frac{\sigma^2_{AD}}{n_m n_d} + \frac{\sigma^2_{WM}}{n_m n_d n_x}. \]

\[ E[ (\hat{\mu} - \mu)^2 ] = \int (\hat{\mu} - \mu)^2 dP(\hat{\mu}) = \]

\[ \int \left( \sum_{i=1}^{n_m} \sum_{j=1}^{n_d} \sum_{k=1}^{n_x} (s_{ijk} - \mu) \right)^2 dP_M(m_i) \bigotimes dP_D(d_{ij}|m_i) \bigotimes dP_S(s_{ijk}|d_{ij}, m_i) = \]

\[ \int \left( \sum_{i=1}^{n_m} \sum_{j=1}^{n_d} \sum_{k=1}^{n_x} (s_{ijk} - \mu) \right)^2 dP_M(m_i) \bigotimes dP_D(d_{ij}|m_i) \bigotimes dP_S(s_{ijk}|d_{ij}, m_i) = \]

\[ \frac{1}{N^2} \int \sum_{i=1}^{n_m} \sum_{j=1}^{n_d} \sum_{k=1}^{n_x} (s_{ijk} - \mu_{m_i} + \mu_{m_i} - \mu) \bigotimes dP_M(m_i) \bigotimes dP_D(d_{ij}|m_i) \bigotimes dP_S(s_{ijk}|d_{ij}, m_i) = \]

\[ \frac{1}{N^2} \int \sum_{i=1}^{n_m} \sum_{j=1}^{n_d} \sum_{k=1}^{n_x} (s_{ijk} - \mu_{m_i} + \mu_{m_i} - \mu) \bigotimes dP_M(m_i) \bigotimes dP_D(d_{ij}|m_i) \bigotimes dP_S(s_{ijk}|d_{ij}, m_i) = \]

\[ \frac{1}{N^2} \int \sum_{i=1}^{n_m} \sum_{j=1}^{n_d} \sum_{k=1}^{n_x} (s_{ijk} - \mu_{m_i} + \mu_{m_i} - \mu) \bigotimes dP_M(m_i) \bigotimes dP_D(d_{ij}|m_i) \bigotimes dP_S(s_{ijk}|d_{ij}, m_i) = \]

\[ \frac{1}{N^2} \int \sum_{i=1}^{n_m} \sum_{j=1}^{n_d} \sum_{k=1}^{n_x} (s_{ijk} - \mu_{m_i} + \mu_{m_i} - \mu) \bigotimes dP_M(m_i) \bigotimes dP_D(d_{ij}|m_i) \bigotimes dP_S(s_{ijk}|d_{ij}, m_i) = \]
Using \((a + b)^2 = a^2 + b^2 + 2ab\) and the linearity of the integral we can break the last integral into three terms which will be analyzed separately:

\[
\frac{1}{N^2}\sum_{i=1}^{n_m}\sum_{j=1}^{n_d}\sum_{k=1}^{n_x}\sum_{i'=1}^{n_m}\sum_{j'=1}^{n_d}\sum_{k'=1}^{n_x}\int \left( \frac{(s_{ijk} - \mu_{m,i})(s_{ij'k'} - \mu_{m,i'}) + (\mu_{m,i} - \mu)(\mu_{m,i'} - \mu)}{a^2} + \frac{(s_{ijk} - \mu_{m,i})(\mu_{m,i'} - \mu) + (s_{ij'k'} - \mu_{m,i'})(\mu_{m,i} - \mu)}{b^2} \right) \\
\left( \frac{dP_M(m_i)}{a} \circ dP_D(d_{ij}\mid m_i) \circ dP_S(s_{ijk}\mid d_{ij}, m_i) \right) \\
\left( \frac{dP_M(m_i')}\circ dP_D(d_{ij'}\mid m_i') \circ dP_S(s_{ij'k'}\mid d_{ij'}, m_i') \right) \\
\left( \frac{dP_M(m_i''\mid d_{ij''}, m_i''\mid d_{ij''}', m_i'')}\ circ dP_D(d_{ij''}\mid m_i'') \circ dP_S(s_{ij'k''}\mid d_{ij''}, m_i'') \right)
\]

Summand I: \(a^2\)

\[
\frac{1}{N^2}\sum_{i=1}^{n_m}\sum_{j=1}^{n_d}\sum_{k=1}^{n_x}\sum_{i'=1}^{n_m}\sum_{j'=1}^{n_d}\sum_{k'=1}^{n_x}\int (s_{ijk} - \mu_{m,i})(s_{ij'k'} - \mu_{m,i'}) \circ dP_M(m_i) \circ dP_D(d_{ij}\mid m_i) \\
\circ dP_S(s_{ijk}\mid d_{ij}, m_i) \circ dP_M(m_i') \circ dP_D(d_{ij'}\mid m_i') \circ dP_S(s_{ij'k'}\mid d_{ij'}, m_i')
\]

At this point we will analyze Summand I for different indices.
\[ i \neq i' \]

Since \((s_{ijk} - \mu_{mi})\) and \((s_{ij'k'} - \mu_{mi'})\) depend on different variables, any addend of Summand I with \(i \neq i'\) can be rewritten as

\[
\frac{1}{N^2} \int (s_{ijk} - \mu_{mi})(s_{ij'k'} - \mu_{mi'}) \prod_{i=1}^{n_m} dP_M(m_i) \prod_{j=1}^{n_d} dP_D(d_{ij}|m_i) \prod_{k=1}^{n_x} dP_S(s_{ijk}|d_{ij}, m_i) \prod_{i'=1}^{n_m} dP_M(m_{i'}) \prod_{j'=1}^{n_d} dP_D(d_{ij'}|m_{i'}) \prod_{k'=1}^{n_x} dP_S(s_{ij'k'}|d_{ij'}, m_{i'}) =
\]

\[
\frac{1}{N^2} \int (s_{ijk} - \mu_{mi}) \prod_{i=1}^{n_m} dP_M(m_i) \prod_{j=1}^{n_d} dP_D(d_{ij}|m_i) \prod_{k=1}^{n_x} dP_S(s_{ijk}|d_{ij}, m_i) \prod_{i'=1}^{n_m} dP_M(m_{i'}) \prod_{j'=1}^{n_d} dP_D(d_{ij'}|m_{i'}) \prod_{k'=1}^{n_x} dP_S(s_{ij'k'}|d_{ij'}, m_{i'}) = \int (s_{ij'k'} - \mu_{mi'}) \prod_{j'=1}^{n_d} dP_D(d_{ij'}|m_{i'}) \prod_{k'=1}^{n_x} dP_S(s_{ij'k'}|d_{ij'}, m_{i'}) = 0 \text{ (by definition)}
\]

\[ i = i', j \neq j' \]

\[
\frac{1}{N^2} \int (s_{ijk} - \mu_{mi})(s_{ij'k'} - \mu_{mi'}) \prod_{i=1}^{n_m} dP_M(m_i) \prod_{j=1}^{n_d} dP_D(d_{ij}|m_i) \prod_{k=1}^{n_x} dP_S(s_{ijk}|d_{ij}, m_i) \prod_{i'=1}^{n_m} dP_M(m_{i'}) \prod_{j'=1}^{n_d} dP_D(d_{ij'}|m_{i'}) \prod_{k'=1}^{n_x} dP_S(s_{ij'k'}|d_{ij'}, m_{i'}) =
\]

\[
= \frac{1}{N^2} \int \left[ \int (s_{ijk} - \mu_{mi}) \prod_{j=1}^{n_d} dP_D(d_{ij}|m_i) \prod_{k=1}^{n_x} dP_S(s_{ijk}|d_{ij}, m_i) \int (s_{ij'k'} - \mu_{mi'}) \prod_{k'=1}^{n_x} dP_S(s_{ij'k'}|d_{ij'}, m_{i'}) \prod_{i=1}^{n_m} dP_M(m_i) \right] = 0 \text{ (by definition)}
\]

\[ i = i', j = j', k \neq k' \]

\[
\frac{1}{N^2} \int (s_{ijk} - \mu_{mi})(s_{ij'k'} - \mu_{mi'}) \prod_{i=1}^{n_m} dP_M(m_i) \prod_{j=1}^{n_d} dP_D(d_{ij}|m_i) \prod_{k=1}^{n_x} dP_S(s_{ijk}|d_{ij}, m_i) \prod_{i'=1}^{n_m} dP_M(m_{i'}) \prod_{j'=1}^{n_d} dP_D(d_{ij'}|m_{i'}) \prod_{k'=1}^{n_x} dP_S(s_{ij'k'}|d_{ij'}, m_{i'}) =
\]

\[
= \frac{1}{N^2} \int \left[ \int (s_{ijk} - \mu_{mi}) \prod_{k=1}^{n_x} dP_S(s_{ijk}|d_{ij}, m_i) \cdot \int (s_{ij'k'} - \mu_{mi'}) \prod_{k'=1}^{n_x} dP_S(s_{ij'k'}|d_{ij'}, m_{i'}) \right] \prod_{j=1}^{n_d} dP_D(d_{ij}|m_i) \prod_{i=1}^{n_m} dP_M(m_i) = \frac{1}{N^2} \int (\mu_{mi} - \mu_{mi})^2 \prod_{i=1}^{n_m} dP_M(m_i) \prod_{j=1}^{n_d} dP_D(d_{ij}|m_i) = \frac{\sigma_{AD}^2}{N^2}. \]
and therefore
\[
\sum_{i=1}^{n_m} \sum_{j=1}^{n_d} \sum_{k=1}^{n_x} \frac{\bar{\sigma}_{AD}^2}{N^2} = \frac{n_m n_d n_x}{N^2} \bar{\sigma}_{AD}^2 = \frac{\bar{\sigma}_{AD}^2}{n_m n_d}.
\]

\[i = i', j = j', k = k'\]

\[
\frac{1}{N^2} \int (s_{ijk} - \mu_{m_i})(s_{ijk} - \mu_{m_i}) n_m \prod_{i=1}^{n_m} dP_M(m_i) \prod_{j=1}^{n_d} dP_D(d_{ij}|m_i) \prod_{k=1}^{n_x} dP_S(s_{ijk}|d_{ij}, m_i) =
\]

\[
= \frac{1}{N^2} \int (s_{ijk} - \mu_{m_i})^2 n_m \prod_{i=1}^{n_m} dP_M(m_i) \prod_{j=1}^{n_d} dP_D(d_{ij}|m_i) \prod_{k=1}^{n_x} dP_S(s_{ijk}|d_{ij}, m_i) = \frac{\sigma_{WM}^2}{N^2},
\]

and thus
\[
\sum_{i=1}^{n_m} \sum_{j=1}^{n_d} \sum_{k=1}^{n_x} \frac{\bar{\sigma}_{WM}^2}{N^2} = \frac{n_m n_d n_x}{N^2} \sigma_{WM}^2 = \frac{\sigma_{WM}^2}{n_m n_d n_x}.
\]

Gathering everything, Summand I amounts to
\[
a^2 = \frac{\bar{\sigma}_{AD}^2}{n_m n_d} + \frac{\sigma_{WM}^2}{n_m n_d n_x}.
\]

**Summand II: \(b^2\)**

\[
\frac{1}{N^2} \sum_{i=1}^{n_m} \sum_{j=1}^{n_d} \sum_{k=1}^{n_x} \sum_{i'=1}^{n_m} \sum_{j'=1}^{n_d} \sum_{k'=1}^{n_x} \int (\mu_{m_i} - \mu)(\mu_{m_{i'}} - \mu) n_m \prod_{i=1}^{n_m} dP_M(m_i) \prod_{j=1}^{n_d} dP_D(d_{ij}|m_i) \prod_{k=1}^{n_x} dP_S(s_{ijk}|d_{ij}, m_i)
\]

\[
\prod_{i'=1}^{n_m} dP_M(m_{i'}) \prod_{j'=1}^{n_d} dP_D(d_{i'j'}|m_{i'}) \prod_{k'=1}^{n_x} dP_S(s_{i'jk'}|d_{i'j'}, m_{i'}) =
\]

\[
= \frac{n_m^2 n_x^2}{N^2} \sum_{i=1}^{n_m} \sum_{i'=1}^{n_m} \int (\mu_{m_i} - \mu)(\mu_{m_{i'}} - \mu) n_m \prod_{i=1}^{n_m} dP_M(m_i) \prod_{i'=1}^{n_m} dP_M(m_{i'})
\]

\[i \neq i'\]

\[
\int (\mu_{m_i} - \mu) n_m \prod_{i=1}^{n_m} dP_M(m_i) \cdot \int (\mu_{m_{i'}} - \mu) n_m \prod_{i'=1}^{n_m} dP_M(m_{i'}) = 0 \text{ (by definition)}
\]

\[i = i'\]

\[
\int (\mu_{m_i} - \mu)^2 n_m \prod_{i=1}^{n_m} dP_M(m_i) = \sigma_{AM}^2.
\]

and therefore
\[
\frac{n_m^2 n_x^2}{N^2} \sum_{i=1}^{n_m} \sigma_{AM}^2 = \frac{\sigma_{AM}^2}{n_m}
\]

Gathering everything Summand II adds to
\[
b^2 = \frac{\sigma_{AM}^2}{n_m}.
\]
Summand III: \(2ab\)

\[
\frac{2}{N^2} \sum_{i=1}^{n_m} \sum_{j=1}^{n_d} \sum_{k=1}^{n_x} \sum_{i'=1}^{n_m} \sum_{j'=1}^{n_d} \sum_{k'=1}^{n_x} \int_{\mathbf{M}} \frac{(s_{ijk} - \mu_m)}{(\mu_{m'} - \mu)} dP_M(m_i) dP_D(d_{ij}|m_i) dP_S(s_{ijk}|d_{ij}, m_i) dP_M(m_{i'}) = 0
\]

(by definition the inmost integral is null)

Gathering all the nonzero terms yields:

\[
\mathbb{E} [(\hat{\mu}_E - \mu)^2] = \frac{\sigma^2_{AM}}{n_m} + \frac{\sigma^2_{AD}}{n_m n_d} + \frac{\sigma^2_{WM}}{n_m n_d n_x}.
\]

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Author contributions

The theorem was proposed by MB; its proof was redacted by AC and revised by the four authors. The document was edited and formatted by AL. The research was directed by MB.

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