Transactions Letters

Improved Sequential Stopping Rule for Monte Carlo Simulation

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Abstract—This letter presents an improved result on the negative-binomial Monte Carlo technique analyzed in a previous paper[1] for the estimation of an unknown probability p. Specifically, the confidence level associated to a relative interval $[p/\mu_2, p\mu_1]$, with μ_1, $\mu_2 > 1$, is proved to exceed its asymptotic value for a broader range of intervals than that given in the referred paper, and for any value of p. This extends the applicability of the estimator, relaxing the conditions that guarantee a given confidence level.

Index Terms—Simulation, Monte Carlo methods, sequential stopping rule.

I. INTRODUCTION

MONTE CARLO (MC) methods are widely used for estimating an unknown parameter by means of repeated trials or realizations of a random experiment. An important particular case is that in which the parameter to be estimated is the probability p of a certain event H, and realizations are independent. In this setting, the technique of negative-binomial MC (NBMC) [1] can be used. This technique applies a sequential stopping rule, which consists in carrying out as many realizations as necessary to obtain a given number N of occurrences of H. Based on this rule, an estimator is introduced in [1], and it is shown to have a number of interesting properties, in the form of respective bounds for its bias, relative precision, and confidence level for a relative interval $[p/\mu_2, p\mu_1]$; μ_1, $\mu_2 > 1$. Specifically, regarding the latter, it is derived in [1] that the confidence level $c = \Pr[p/\mu_2 \leq \hat{p} \leq p\mu_1]$ has an asymptotic value $\bar{c}$ as $p \to 0$, given by[2]

$$\bar{c} = \gamma(N, (N-1)\mu_2) - \gamma\left(N, \frac{N-1}{\mu_1}\right). \quad (1)$$

Furthermore, the confidence level c is assured to exceed $\bar{c}$ for

$$\mu_2 \geq \frac{N + \sqrt{N}}{N - 1}, \quad \mu_1 \geq \frac{N - 1}{N - \sqrt{\frac{3}{2}N}}, \quad (2)$$

[1]L. Mendo and J. M. Hernando, "A simple sequential stopping rule for Monte Carlo simulation," *IEEE Trans. Commun.*, vol. 54, no. 2, pp. 231–241, Feb. 2006.

[2]$\gamma(r, x)$ denotes the incomplete gamma function, defined as $\gamma(r, x) = 1/\Gamma(r) \cdot \int_0^x e^{-t}t^{r-1}dt$.

provided that[3]

$$p < \frac{N - 1}{\lceil \frac{7}{2}N - 1 \rceil \mu_1}. \quad (3)$$

In this letter, the sufficient conditions that assure a confidence level $c > \bar{c}$ for the NBMC estimator are relaxed in two ways:

- The restriction on p given by (3) is eliminated, i.e. p can be an unconstrained value between 0 and 1.
- The condition for μ_1 given by (2) is weakened, while maintaining the condition for μ_2. Thus μ_1 can be further decreased while having the same guaranteed confidence level given by (1).

The result is presented in Section II, and conclusions are given in Section III.

II. RESULT

Consider a random experiment, and an event H associated to that experiment (more generally, there may be a set of events associated to the experiment, one of which is of interest). The probability p of event H is to be estimated from independent realizations of the experiment, using the method described in [1]. Specifically, given[4] $N \in \mathbb{N}$, with $N \geq 3$, realizations are carried out until N occurrences of H are obtained. The number of realizations is thus a negative-binomial random variable[5] $\boldsymbol{n}$, from which p is estimated as [1]

$$\hat{p} = \frac{N - 1}{\boldsymbol{n}}. \quad (4)$$

For μ_1, $\mu_2 > 1$ given, consider the interval $[p/\mu_2, p\mu_1]$, and its associated confidence $c = \Pr[p/\mu_2 \leq \hat{p} \leq p\mu_1]$. As shown in [1], c tends to $\bar{c}$ given by (1) as $p \to 0$.

Proposition 1: For any $p \in (0, 1)$, with $\hat{p}$ given by (4), the lower bound $c > \bar{c}$ holds if

$$\mu_2 \geq \frac{N + \sqrt{N}}{N - 1}, \quad \mu_1 \geq \frac{N - 1}{N - \frac{1}{2} - \sqrt{N - \frac{1}{2}}}. \quad (5)$$

Proof: Consider $N \geq 3$, μ_1, $\mu_2 > 1$, and $p \in (0, 1)$. Let us define

$$n_1 = \left\lceil \frac{N - 1}{p\mu_1} \right\rceil \quad (6)$$

$$n_2 = \left\lfloor \frac{(N - 1)\mu_2}{p} \right\rfloor. \quad (7)$$

[3]$\lfloor \cdot \rfloor$ and $\lceil \cdot \rceil$ respectively denote rounding to the nearest integer towards $-\infty$ and towards ∞.

[4]$\mathbb{N}$ denotes the set of natural numbers, $\{1, 2, \dots\}$.

[5]Random variables are denoted in boldface throughout the letter.

The confidence c is given by $1 - c_1 - c_2$ with[6]

$$c_1 = \Pr[\boldsymbol{n} \leq n_1 - 1]$$
$$= \frac{p^N}{(N-1)!} \sum_{n=N}^{n_1-1} (n-1)^{(N-1)}(1-p)^{n-N}, \quad (8)$$

$$c_2 = \Pr[\boldsymbol{n} \geq n_2 + 1]$$
$$= \frac{p^N}{(N-1)!} \sum_{n=n_2+1}^{\infty} (n-1)^{(N-1)}(1-p)^{n-N}. \quad (9)$$

Let $\bar{c}_1$ and $\bar{c}_2$ be respectively defined as $\lim_{p \to 0} c_1$ and $\lim_{p \to 0} c_2$. From [1, appendix C], $\bar{c}_1 = \gamma(N, (N-1)/\mu_1)$ and $\bar{c}_2 = 1 - \gamma(N, (N-1)\mu_2)$. We will show that $\bar{c}_1 > c_1$ and $\bar{c}_2 > c_2$ for μ_1, μ_2 as in (5). This will establish[7] that $c > \bar{c}$.

The inequality $\bar{c}_2 > c_2$ is equivalent to $\Pr[\boldsymbol{n} \leq n_2] > \lim_{p \to 0} \Pr[\boldsymbol{n} \leq n_2]$, which is established in [1, appendix C] for μ_2 as in (5) and n_2 given by (7).

In order to show that $\bar{c}_1 > c_1$, we first note that

$$\bar{c}_1 = \gamma\left(N, \frac{N-1}{\mu_1}\right) = \frac{p^N}{(N-1)!} \int_0^{\frac{N-1}{p\mu_1}} t^{N-1} e^{-pt} dt$$
$$> \frac{p^N}{(N-1)!} \int_{N-1}^{n_1-1} t^{N-1} e^{-pt} dt. \quad (10)$$

Lemma 1 given in the Appendix implies that the right-hand side of (10) will be greater than or equal to that of (8) if $n_1 - 1 \leq (N - 1/2 - \sqrt{N-1/2})/p + 1/2$. From (6), n_1 is upper bounded by $(N-1)/(p\mu_1) + 1$. Therefore, in order to assure that $\bar{c}_1 > c_1$ it is sufficient that

$$\frac{N-1}{p\mu_1} \leq \frac{N - \frac{1}{2} - \sqrt{N - \frac{1}{2}}}{p} + \frac{1}{2}, \quad (11)$$

or equivalently

$$\mu_1 \geq \frac{N-1}{N - \frac{1}{2} - \sqrt{N - \frac{1}{2}} + \frac{p}{2}}. \quad (12)$$

Since $p > 0$, (12) holds for μ_1 as in (5). ∎

This result removes some of the restrictions that are used in [1] to assure that $c > \bar{c}$. Specifically, p can take any value, and the minimum required value for μ_1 is lower.

For the particular case that $\mu_1 = \mu_2 = 1 + m$, where $m > 0$ is a relative error margin, it is easily seen that the limiting condition in (5) is that for μ_2, i.e.

$$m \geq \frac{\sqrt{N}+1}{N-1}. \quad (13)$$

The dashed curves in Fig. 1 depict the guaranteed confidence $\bar{c}$ (given by (1)) as a function of N and m, for m within the allowed range (13). The solid line represents the minimum confidence $\bar{c}_{\min}$ that can be guaranteed as a function of m. This corresponds to the lowest N permitted by (13) for a given m; increasing N gives larger guaranteed confidence levels.

The achievable region in the $(m, \bar{c})$ plane is that above the solid curve, in the following sense: for any $(m, \bar{c})$ within this
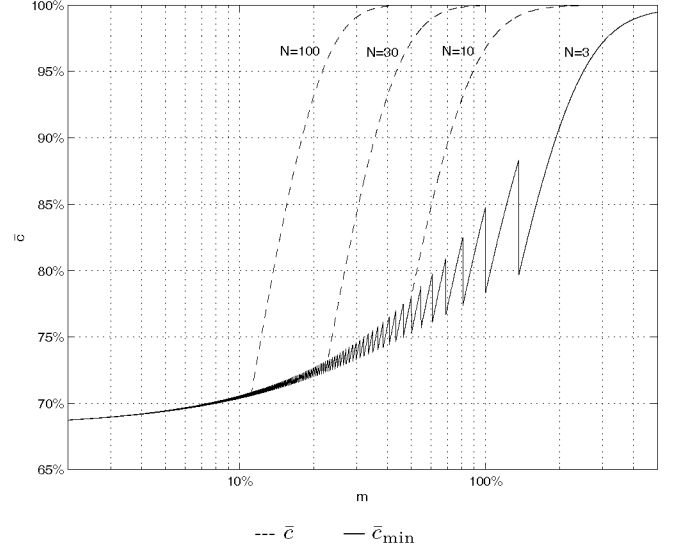

Fig. 1.   Guaranteed confidence $\bar{c}$ and minimum confidence that can be guaranteed $\bar{c}_{\min}$.

region, the confidence level associated to the error margin m can be assured to be greater than $\bar{c}$, irrespective of p; this is accomplished by selecting N according to (1) (or, equivalently, using the curves in [1, fig. 5(a)]). Comparing with [1, fig. 4], it is seen that Proposition 1 enlarges the achievable region, specially for low m; besides, it removes the restriction on p. Fig. 1 thus replaces [1, fig. 4(a)]; and [1, figures 4(b) and 5(b)] are no longer necessary.

As an example, consider the following problem: given an NBMC estimator $\hat{p}$ of an unknown p with $N = 30$, find the minimum m such that $\Pr[p/(1+m) \leq \hat{p} \leq p(1+m)] > 75\%$. From Proposition 1 and (1), $m = 23.7\%$. The results in [1], on the contrary, can only give $m = 24.5\%$, since $(23.7\%, 75\%)$ is not in the achievable region according to [1, fig. 4(a)]; besides, $p < 0.224$ is required.

III. Conclusions

In this letter, the statistical characterization of the NBMC estimator introduced in [1] has been improved by relaxing the conditions that guarantee a certain confidence level. It has been established that, for $p \in (0, 1)$ arbitrary, the NBMC estimator has a confidence level better than (1) provided that μ_1, μ_2 satisfy (5). This result extends the range of application of the NBMC estimation technique.

Appendix

The following lemma, used in the proof of proposition 1, is now established.

Lemma 1: Given $N, n^* \in \mathbb{N}$ with $N \geq 3$ and

$$n^* \leq \frac{N - \frac{1}{2} - \sqrt{N - \frac{1}{2}}}{p} + \frac{1}{2} \quad (14)$$

the following inequality holds:

$$\int_{N-1}^{n^*} n^{N-1} e^{-pn} dn \geq \sum_{n=N}^{n^*} (n-1)^{(N-1)}(1-p)^{n-N}. \quad (15)$$

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[6]The following notation is used: $k^{(i)} = k(k-1) \cdots (k-i+1)$, $k^{(0)} = 1$.

[7]It should be noted that, although [1, appendix C] considers $n_2 \geq a$, the actual range of values for n_2 is $n_2 > a - 1$. Nonetheless, the proofs in [1, appendix C] can be readily generalized to $n_2 > a - 1$.
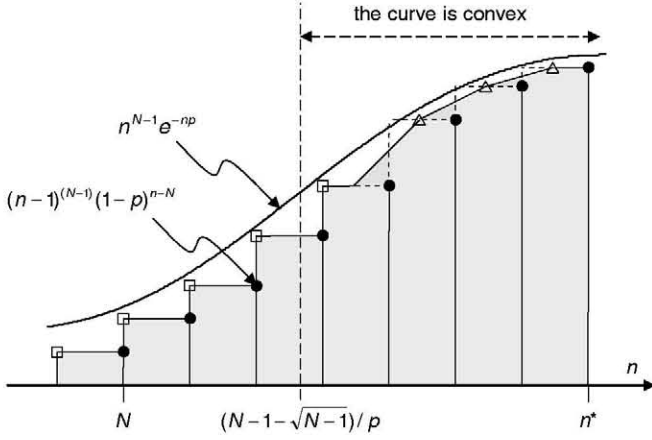
Fig. 2.   Graphical representation for the proof of Lemma 1.

Proof: We first note that the sub-integral function is increasing for $n < (N-1)/p$, and is convex for $(N-1-\sqrt{N-1})/p < n < (N-1)/p$. As figure 2 illustrates, each term of the sum in (15) can be identified with the area of a rectangle of unit width. Specifically, the term corresponding to a given n is associated to the rectangle that extends horizontally from $n-1$ to n in the figure. In addition, for the rectangles situated to the right of $(N-1-\sqrt{N-1})/p$ (where the sub-integral function is convex), the flat tops are replaced by straight lines joining the centers, without altering the total area. The inequality (15) will hold if the area below the curve in the interval $(N-1, n^*)$ is larger than the shaded area in the figure. We divide this interval in two: $(N-1, (N-1-\sqrt{N-1})/p)$ and $((N-1-\sqrt{N-1})/p, n^*)$, and require that in each of these intervals the area of the curve be larger than the part of the shaded area corresponding to that interval. In the first interval, since the curve is increasing, it suffices that the curve be above the square marks for $n \leq \lfloor (N-1-\sqrt{N-1})/p \rfloor$, as shown in the figure. In the second interval, since the curve is increasing and convex, it suffices that the curve be above the square mark located at $\lfloor (N-1-\sqrt{N-1})/p \rfloor + 1$ and above the triangle marks. As a result, to establish (15) it is sufficient that

(i) the sub-integral function be above the square marks for $N \leq n \leq (N-1-\sqrt{N-1})/p + 1$; and
(ii) the sub-integral function be above the triangle marks for $(N-1-\sqrt{N-1})/p + 1 < n < n^*$.

We analyze these conditions separately.

(i) With x defined as

$$x = \frac{1}{p} \ln \frac{(n-1)^{N-1} e^{-(n-1)p}}{(n-1)^{(N-1)}(1-p)^{n-N}}$$
$$= -\frac{1}{p} \sum_{i=1}^{N-1} \ln\left(1 - \frac{i-1}{n-1}\right) - \frac{n-N}{p}\ln(1-p) - (n-1), \quad (16)$$

condition (i) is expressed as $x \geq 0$ for $n \leq (N-1-\sqrt{N-1})/p + 1$. Defining $M = N-1$ and $\nu = (n-1)p$,

$$x = -\frac{1}{p}\sum_{i=1}^{N-1}\ln\left(1 - \frac{(i-1)p}{\nu}\right) - \frac{1}{p}\left(\frac{\nu}{p} - M\right)\ln(1-p) - \frac{\nu}{p}. \quad (17)$$

Using the Taylor expansion $\ln(1-t) = -\sum_{j=1}^{\infty} t^j/j$, $|t| < 1$, (17) is transformed into $x = \sum_{j=0}^{\infty} x_j p^j$ with

$$x_j = \frac{1}{(j+1)\nu^{j+1}}\sum_{i=1}^{N-1}(i-1)^{j+1} + \frac{\nu}{j+2} - \frac{M}{j+1}. \quad (18)$$

The term x_0 is easily seen to be nonnegative for $\nu \leq M - \sqrt{M}$, i.e. for $n \leq (N-1-\sqrt{N-1})/p + 1$. We now prove that the remaining coefficients x_j, $j \geq 1$ are also nonnegative for $\nu \leq M - \sqrt{M}$.

We begin with the case $N \geq 5$, $j \geq 2$. Using the inequality

$$\sum_{i=1}^{N-1}(i-1)^{j+1} > \int_{1}^{N-1}(i-1)^{j+1}di$$
$$= \frac{(N-2)^{j+2}}{j+2} = \frac{(M-1)^{j+2}}{j+2} \quad (19)$$

in (18), we can bound

$$x_j > \frac{(M-1)^{j+2} + (j+1)\nu^{j+2} - (j+2)M\nu^{j+1}}{(j+1)(j+2)\nu^{j+1}}. \quad (20)$$

The denominator in (20) is positive. Let y_j denote the numerator. We compute

$$\frac{\partial y_j}{\partial \nu} = (j+2)(j+1)(\nu - M)\nu^j < 0, \quad (21)$$

from which it suffices to consider $\nu = M - \sqrt{M}$. Expressing

$$y_j|_{\nu = M - \sqrt{M}} = M^{j+2}\left(1 - \frac{1}{\sqrt{M}}\right)^{j+1}$$
$$\cdot \left[\left(1 - \frac{1}{\sqrt{M}}\right)\left(1 + \frac{1}{\sqrt{M}}\right)^{j+2}\right. \quad (22)$$
$$\left. + (j+1)\left(1 - \frac{1}{\sqrt{M}}\right) - (j+2)\right]$$

and denoting the bracketed term by Y_j, we now compute the following partial derivatives as if j were a continuous variable:

$$\frac{\partial Y_j}{\partial j} = \left(1 - \frac{1}{\sqrt{M}}\right)\left(1 + \frac{1}{\sqrt{M}}\right)^{j+2}$$
$$\cdot \ln\left(1 + \frac{1}{\sqrt{M}}\right) - \frac{1}{\sqrt{M}} \quad (23)$$

$$\frac{\partial^2 Y_j}{\partial j^2} = \left(1 - \frac{1}{\sqrt{M}}\right)\left(1 + \frac{1}{\sqrt{M}}\right)^{j+2}\ln^2\left(1 + \frac{1}{\sqrt{M}}\right). \quad (24)$$

The right-hand side of (24) is positive, and using the inequality $\ln(1+t) > t - t^2/2$ we can bound (23) for $j = 2$ as

$$\frac{\partial Y_j}{\partial j}\bigg|_{j=2} = \left(1 - \frac{1}{\sqrt{M}}\right)\left(1 + \frac{1}{\sqrt{M}}\right)^4\frac{1}{\sqrt{M}}$$
$$\cdot \left(1 - \frac{1}{2\sqrt{M}}\right) - \frac{1}{\sqrt{M}} > 0. \quad (25)$$

Therefore the right-hand side of (23) is positive for $j \geq 2$. Consequently, in order to establish that $y_j \geq 0$, it suffices to show that $Y_2 \geq 0$. Defining $m = 1/\sqrt{M}$, Y_2 can be expressed as $-m^2(m^3 + 3m^2 + 2m - 2)$. According to Descartes' sign rule, this polynomial has only one positive root. For $m \to \infty$ the polynomial takes negative values, and for $m = 1/2$ it is

positive. Therefore, it is positive for $m \leq 1/2$, i.e. for $M \geq 4$, or $N \geq 5$.

For $N = 4$, $j \geq 2$, we have

$$x_j = \frac{(j+2)(1 + 2^{j+1}) + (j+1)\nu^{j+2} - 3(j+2)\nu^{j+1}}{(j+2)(j+1)\nu^{j+1}} \quad (26)$$

Let z_j denote the numerator in (26). Since

$$\frac{\partial z_j}{\partial \nu} = (j+2)(j+1)\nu^j(\nu - 3) < 0, \quad (27)$$

it suffices to consider $\nu = 3 - \sqrt{3}$. Bounding z_j as

$$z_j > (j+2)(2^{j+1} - 3\nu^{j+1}) + (j+1)\nu^{j+2}, \quad (28)$$

$z_j|_{\nu=3-\sqrt{3}}$ is seen to be positive for $j \geq 2$.

For $N = 3$, $j \geq 2$,

$$x_j = \frac{j + 2 + (j+1)\nu^{j+2} - 2(j+2)\nu^{j+1}}{(j+2)(j+1)\nu^{j+1}}, \quad (29)$$

and similar arguments to those for $N = 4$, $j \geq 2$ show that $x_j > 0$.

For $N \geq 3$, $j = 1$, using the identity

$$\sum_{i=1}^{N-1}(i-1)^2 = \frac{(N-2)^3}{3} + \frac{(N-2)^2}{2} + \frac{N-2}{6}$$
$$= \frac{(M-1)^3}{3} + \frac{(M-1)^2}{2} + \frac{M-1}{6} \quad (30)$$

we obtain from (18)

$$x_j = \frac{4\nu^3 - 6M\nu^2 + 2(M-1)^3 + 3(M-1)^2 + M - 1}{12\nu^2}. \quad (31)$$

From Descartes' sign rule, the numerator of (31) considered as a polynomial in ν has two positive roots at most. This polynomial is positive for $\nu = 0$ and for $\nu \to \infty$, and negative for $\nu = M$. Thus, it will be positive for $\nu \leq M - \sqrt{M}$ if it is for $\nu = M - \sqrt{M}$. Substituting this ν and defining $m = \sqrt{M}$, the numerator is expressed as $m^2(3m^2 - 4m + 1)$, which is positive for $m > 1$, or equivalently $M > 1$, and thus for $N \geq 3$.

(ii) With x' defined as

$$x' = \frac{1}{p} \ln \frac{\left(n - \frac{1}{2}\right)^{N-1} e^{-\left(n - \frac{1}{2}\right)p}}{(n-1)^{(N-1)}(1-p)^{n-N}}$$
$$= -\frac{1}{p}\sum_{i=1}^{N-1}\ln\left(1 - \frac{i - \frac{1}{2}}{n - \frac{1}{2}}\right) \quad (32)$$
$$- \frac{n-N}{p}\ln(1-p) - \left(n - \frac{1}{2}\right),$$

and taking into account (14), in order to fulfil condition (ii) it is sufficient that $x' \geq 0$ for $n \leq (N-1/2-\sqrt{N-1/2})/p+1/2$. Defining $M' = N - 1/2$ and $\nu' = (n - 1/2)p$,

$$x' = -\frac{1}{p}\sum_{i=1}^{N-1}\ln\left(1 - \frac{\left(i - \frac{1}{2}\right)p}{\nu'}\right)$$
$$- \frac{1}{p}\left(\frac{\nu'}{p} - M'\right)\ln(1-p) - \frac{\nu'}{p}. \quad (33)$$

Proceeding as with x, we can express $x' = \sum_{j=0}^{\infty} x'_j p^j$ with

$$x'_j = \frac{1}{(j+1)\nu'^{j+1}}\sum_{i=1}^{N-1}\left(i - \frac{1}{2}\right)^{j+1} + \frac{\nu'}{j+2} - \frac{M'}{j+1}. \quad (34)$$

x'_0 is seen to be nonnegative for $\nu' \leq M' - \sqrt{M' - 1/4}$, and thus for $\nu' \leq M' - \sqrt{M'}$, i.e. for $n \leq (N - 1/2 - \sqrt{N - 1/2})/p + 1/2$. We now prove that the remaining coefficients x'_j, $j \geq 1$ are also nonnegative for $\nu' \leq M' - \sqrt{M'}$.

We begin with the case $N \geq 5$, $j \geq 2$. Using the inequality

$$\sum_{i=1}^{N-1}\left(i - \frac{1}{2}\right)^{j+1} > \int_{1/2}^{N-1}\left(i - \frac{1}{2}\right)^{j+1} di$$
$$= \frac{\left(N - \frac{3}{2}\right)^{j+2}}{j+2} = \frac{(M'-1)^{j+2}}{j+2} \quad (35)$$

in (34), we can bound

$$x'_j > \frac{(M'-1)^{j+2} + (j+1)\nu'^{j+2} - (j+2)M'\nu'^{j+1}}{(j+1)(j+2)\nu'^{j+1}}. \quad (36)$$

The denominator in (36) is positive, and the numerator is as that in (20) with M replaced by M' and ν replaced by ν'. It stems that $x'_j > 0$ for $M' \geq 4$, i.e. $N \geq 5$, and $j \geq 2$.

For $N = 4$, $j \geq 2$, (34) gives

$$x'_j = \left[(j+2)\left(\left(\tfrac{1}{2}\right)^{j+1} + \left(\tfrac{3}{2}\right)^{j+1} + \left(\tfrac{5}{2}\right)^{j+1}\right) + (j+1)\nu'^{j+2} \right.$$
$$\left. - \tfrac{7}{2}(j+2)\nu'^{j+1}\right] / \left[(j+2)(j+1)\nu'^{j+1}\right], \quad (37)$$

which is shown to be positive with analogous arguments as for x_j.

For $N = 3$, $j \geq 2$,

$$x'_j = \left[(j+2)\left(\left(\tfrac{1}{2}\right)^{j+1} + \left(\tfrac{3}{2}\right)^{j+1}\right) + (j+1)\nu'^{j+2} \right.$$
$$\left. - \tfrac{5}{2}(j+2)\nu'^{j+1}\right] / \left[(j+2)(j+1)\nu'^{j+1}\right], \quad (38)$$

and similarly it is shown to be positive.

For $N \geq 3$, $j = 1$, using the identity

$$\sum_{i=1}^{N-1}\left(i - \frac{1}{2}\right)^2 = \frac{\left(N - \frac{3}{2}\right)^3}{3} + \frac{\left(N - \frac{3}{2}\right)^2}{2} + \frac{N - \frac{3}{2}}{6}$$
$$= \frac{(M'-1)^3}{3} + \frac{(M'-1)^2}{2} + \frac{M'-1}{6} \quad (39)$$

we obtain an expression for x'_j which coincides with (31) replacing M by M' and ν by ν'. Therefore, x'_j is positive for $M' > 1$, and thus for $N \geq 3$.

According to the foregoing, conditions (i) and (ii) hold for $N \geq 3$. This establishes the stated result (15). ∎

REFERENCES

[1] L. Mendo and J. M. Hernando, "A simple sequential stopping rule for Monte Carlo simulation," *IEEE Trans. Commun.*, vol. 54, no. 2, pp. 231–241, Feb. 2006.