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Cost of Splitting in Monte Carlo Transport

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COST OF SPLITTING IN MONTE CARLO TRANSPORT

by

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ABSTRACT

In a simple transport problem designed to estimate transmission through a plane slab of X free paths by Monte Carlo methods, it is shown that m -splitting ($m > 2$) does not pay unless $e^X > m(m+3)/(m-1)$. In such a case, the minimum total cost in terms of machine time is obtained as a function of m , and the optimal value of m is determined.

I. INTRODUCTION

If an elementary experiment can result in $m+1$ different ways: $i=0, \dots, m$, the i 'th way having probability $p(i)$ and an assigned "weight" $x(i)$, then

$$\bar{x} = \sum_{i=0}^m x(i) p(i)$$

is called the "expected value" of x , and

$$V = \overline{x^2} - \bar{x}^2$$

its "variance," where $\overline{x^2} = \sum_{i=0}^m x^2(i) p(i)$.

In such a case, the central limit theorem asserts that, in a large number N of such experiments,

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$$P \left\{ \left| \frac{\left(\sum_{\tau=1}^N x(i_{\tau})/N \right) - \bar{x}}{\bar{x}} \right| < z \cdot \frac{\sqrt{V/N}}{\bar{x}} \right\} \cong \frac{2}{\sqrt{2\pi}} \int_0^z e^{-t^2/2} dt .$$

The probability P here means $\sum p(i_1) \cdots p(i_N)$ summed over all those N -tuples $(i_1, \dots, i_N)$ for which the sum $x(i_1) + \cdots + x(i_N)$ satisfies the stated inequality.

The fraction $E = \frac{\sqrt{V/N}}{\bar{x}}$ is called the "relative error" of the mean $\bar{x}$.

In Monte Carlo transport problems one is concerned with the estimation of such a mean $\bar{x}$ by processing a large number N of source particles. Each of the N "histories" may be regarded as the trial τ of an elementary experiment contributing a certain weight $x(i_{\tau})$ to a definite counter with some probability $p(i_{\tau})$. Obviously the practical question is the choice of a method of sampling which minimizes the total cost C of processing a fixed number N of source particles, with a stipulated error E . To make the ideas and notation clear, we list the essential parameters.

N = number of source particles

$\bar{x}$ = expected value of x (method independent, necessarily)

V = variance of x (method dependent)

$E = (V/N)^{1/2}/\bar{x}$, stipulated error (method independent)

c = cost per source particle (method dependent)

$C = cN$ total cost of method (method dependent)

We seek a method for which C is minimal. Since $C = cN = c(V/E^2 \bar{x}^2)$ where $E^2 \bar{x}^2$ is method independent, we need only minimize the "cost function"

$$f = cV ,$$

where both factors are method dependent. Note that the number N of particles is irrelevant.

II. A SIMPLE TRANSPORT PROBLEM

We obtain such an optimal method for the following simple problem, the objective being determination of the expected transmission $\bar{x}$.

- a. Source particles enter plane slab normal to surface.
- b. Collision results in total absorption.
- c. Slab X free paths thick.
- d. c_0 = cost of computing one distance-to-collision (infinite medium) and comparison with distance to boundary.

As options we consider the following methods:

Method I. No splitting.

Method II. Splitting each source particle into $m \geq 2$ particles, each of weight $1/m$, at entrance.

Method III. Such splitting at distance x from entrance, $0 < x < X$.

III. TOTAL COST OF THE METHODS

In Method I (see Fig. 1), with no splitting, the elementary experiment is a hit ($i=1$) or miss ($i=0$) situation, with

$$\begin{aligned} p(1) &= e^{-X} \equiv p & x(1) &= 1 \\ p(0) &= q = 1-p & x(0) &= 0 \end{aligned}$$

in the notation of Sec. I. (We use the notation $p = e^{-X}$ throughout.) Hence

$$c = c_0$$

$$\bar{x} = p$$

$$\overline{x^2} = p$$

$$V = p - p^2 = pq$$

$$f_I = cV = c_0 pq$$

Fig. 1. Method I.

In Method II, with 1-to- m splitting at $x=0$, there are $m+1$ possible outcomes to an elementary experiment, namely the arrival at $x=X$ of i tracks, $i=0, 1, \dots, m$. Here we have

$$p(i) = \binom{m}{i} q^{m-i} p^i, \quad x(i) = (i/m) \quad i=0, \dots, m,$$

$$c = mc_0$$

$$\begin{aligned}\bar{x} &= \sum_0^m (i/m) \binom{m}{i} q^{m-i} p^i = \sum_1^m \binom{m-1}{i-1} q^{m-i} p^i \\ &= \left(\sum_0^{m-1} \binom{m-1}{i} q^{m-1-i} p^i \right) p = (q+p)^{m-1} p = p\end{aligned}$$

$$\begin{aligned}\bar{x}^2 &= \sum_0^m (i/m)^2 \binom{m}{i} q^{m-i} p^i = \sum_1^m (i/m) \binom{m-1}{i-1} q^{m-i} p^i \\ &= (p/m) \sum_0^{m-1} (i+1) \binom{m-1}{i} q^{m-1-i} p^i = \frac{p}{m} \{ (m-1)p + 1 \} \\ &= p^2 + \frac{1}{m} (p - p^2) = p^2 + pq/m\end{aligned}$$

$$V = pq/m$$

$$f_{III} = (mc_0) (pq/m) = c_0 pq.$$

Hence, compared with Method I, Method II m -tuples the cost per particle, and cuts the variance by m , leaving the function f unchanged.

In Method III with m -splitting at x , $0 < x < X$ in case of arrival at x , there are the same $m+1$ possibilities as in Method II, but now

$$p(0) = 1 - e^{-x} + e^{-x} Q^m, \quad x(0) = 0.$$

$$p(i) = e^{-x} \binom{m}{i} Q^{m-i} P^i, \quad x(i) = (i/m), \quad i=1, \dots, m,$$

$$\text{where } P = e^{-(X-x)} = e^x p \text{ and } Q = 1 - P.$$

Using the results of Method II in the summations, with P, Q replacing p, q , we obtain for this method

$$c = c_0 + e^{-x} (mc_0) = c_0 (1 + me^{-x})$$

$$\bar{x} = \sum_0^m x(i) p(i) = e^{-x} \sum_1^m (i/m) \binom{m}{i} Q^{m-i} p^i$$

$$= e^{-x} p = p$$

$$\overline{x^2} = \sum_0^m x^2(i) p(i) = e^{-x} \sum_1^m (i/m)^2 \binom{m}{i} Q^{m-i} p^i$$

$$= e^{-x} (p^2 + PQ/m) = p (p + \frac{1-p}{m}) = \frac{p}{m} (1 + (m-1) p e^x)$$

$$= p^2 \left\{ \frac{1}{mp} + \frac{m-1}{m} e^x \right\}$$

$$V = p^2 \left\{ \left(\frac{1}{mp} - 1 \right) + \frac{m-1}{m} e^x \right\}$$

$$f(x) = c_0 p^2 (1 + m e^{-x}) \left\{ \left(\frac{1}{mp} - 1 \right) + \frac{m-1}{m} e^x \right\}$$

$$= c_0 p^2 \left\{ \left(\frac{1}{mp} + (m-2) \right) + \frac{m-1}{m} e^x + \left(\frac{1}{p} - m \right) e^{-x} \right\}, 0 < x < X. \quad (1)$$

This indicates the total cost of splitting at an internal surface x free paths from entry, as compared with $f_I = c_0 p q$ of Method I.

IV. CASE OF INCREASING $f(x)$ IN METHOD III

From (1) we see that the derivative

$$f'(x) = c_0 p^2 \left\{ \frac{m-1}{m} e^x - \left(\frac{1}{p} - m \right) e^{-x} \right\}$$

$$= c_0 p^2 e^{-x} \left\{ \frac{m-1}{m} e^{2x} - \frac{1}{p} + m \right\}. \quad (2)$$

Hence, if $e^X = \frac{1}{p} \leq m + \frac{m-1}{m}$, then

$$f'(x) > c_0 p^2 e^{-x} \left\{ \frac{m-1}{m} - \frac{1}{p} + m \right\} \geq 0, 0 < x < X,$$

$f(x)$ is strictly increasing, and from (1)

$$\begin{aligned}\lim_{x \rightarrow 0^+} f(x) &= c_0 p^2 \left\{ \frac{1}{mp} + (m-2) + \frac{m-1}{m} + \frac{1}{p} - m \right\} \\ &= c_0 p^2 \left\{ \frac{m+1}{m} \frac{1}{p} - \frac{m+1}{m} \right\} = \frac{m+1}{m} c_0 p q = \frac{m+1}{m} f_I > f_I.\end{aligned}$$

Hence, if $e^X \leq m + \frac{m-1}{m}$, splitting never pays.

V. CASE OF $f(x)$ CONCAVE-UP IN METHOD III

We now assume $e^X = \frac{1}{p} > m + \frac{m-1}{m}$. In such a case, we see from (2) that

$$\begin{aligned}f'(0) &= c_0 p^2 \left\{ \frac{m-1}{m} - \frac{1}{p} + m \right\} < 0 \\ f'(X) &= c_0 p^2 e^{-X} \left\{ \frac{m-1}{m} e^{2X} - e^X + m \right\} > 0\end{aligned}$$

(since the quadratic has discriminant $b^2 - 4ac = 1 - 4(m-1) = 5 - 4m < 0$ for $m \geq 2$).

Moreover

$$f''(x) = c_0 p^2 \left\{ \frac{m-1}{m} e^x + \left(\frac{1}{p} - m \right) e^{-x} \right\} > 0, \text{ since } \frac{1}{p} > m + \frac{m-1}{m} > m.$$

Hence $f(x)$ has a minimum at a unique x_0 where from (2), $e^{2x_0} = \frac{m}{m-1} \left(\frac{1}{p} - m \right)$;

$$0 < x_0 < X. \quad (3)$$

Thus there is a possibility that $f(x_0)$ might be less than f_I in this case.

We next compute from (1), the minimal value

$$\begin{aligned}f(x_0) &= c_0 p^2 e^{x_0} \left\{ \left(\frac{1}{mp} + (m-2) \right) e^{-x_0} + \frac{m-1}{m} + \left(\frac{1}{p} - m \right) e^{-2x_0} \right\} \\ &= c_0 p^2 e^{x_0} \left\{ \left(\frac{1}{mp} + (m-2) \right) e^{-x_0} + \frac{m-1}{m} + \frac{m-1}{m} \right\} \\ &= c_0 p^2 \left\{ \left(\frac{1}{mp} + (m-2) \right) + 2 \frac{m-1}{m} e^{x_0} \right\}\end{aligned}$$

$$= c_0 p \left\{ \frac{1}{m} + (m-2)p + 2p \left(\frac{m-1}{m} \left(\frac{1}{p} - m \right) \right)^{1/2} \right\} \quad (4)$$

This is the minimal cost of m-splitting in the case $e^X = \frac{1}{p} > m + \frac{m-1}{m}$.

To compare this with f_1 , we consider the ratio

$$\rho = f(x_0)/c_0 p q = \frac{\frac{1}{m} + (m-2)p + 2p \left(\frac{m-1}{m} \left(\frac{1}{p} - m \right) \right)^{1/2}}{1-p} \quad (5)$$

It is easy to verify the equivalence of the following relations:

$$\rho < 1$$

$$\frac{1}{m} + (m-2)p + 2p \left(\frac{m-1}{m} \left(\frac{1}{p} - m \right) \right)^{1/2} < 1-p$$

$$2 \left(\frac{m-1}{m} \left(\frac{1}{p} - m \right) \right)^{1/2} < \frac{m-1}{m} \left(\frac{1}{p} - m \right)$$

$$0 < \left(\frac{m-1}{m} \right)^2 \left(\frac{1}{p} - m \right) \left(\frac{1}{p} - \frac{m(m+3)}{m-1} \right)$$

Hence, for $e^X \equiv \frac{1}{p} > m + \frac{m-1}{m}$, m-splitting at the optimal place x_0 costs less than Method I iff

$$\underline{e^X \equiv \frac{1}{p} > \frac{m(m+3)}{m-1}}$$

(Note that $m(m+3)/(m-1) > m + \frac{m-1}{m}$)

For fixed m, and $X \rightarrow \infty$, $p = e^{-X} \rightarrow 0$, one sees from (5) that $\rho \rightarrow 1/m$.

VI. THE OPTIMAL VALUE OF m

So far, we have held $m \geq 2$ fixed, and shown that m-splitting at the optimal position x_0 pays iff the number X of slab free paths is sufficiently large, namely

$$e^X \equiv 1/p > m(m+3)/(m-1) \equiv R(m) .$$

The function $R(m)$ has the values

m	$R(m)$
2	10
3	9
4	9 1/3
5	10
6	10 4/5

with minimum 9 at $m=3$. Hence, given X we have the cases; for $\frac{1}{p} \equiv e^X$,

1. $1/p \leq 9$, splitting never pays.
2. $9 < 1/p \leq 9 \frac{1}{3}$, only $m=3$ pays.
3. $9 \frac{1}{3} < 1/p \leq 10$, only $m=3$ and $m=4$ pay.
4. $10 < 1/p$, $m = 2, 3, 4, 5$ pay, as well as any other m for which $m(m+3)/(m-1) < 1/p$.

Hence for any given X , the set of integers $m \geq 2$ for which m -splitting pays is well defined, and the remaining problem is to determine which m of this set yields a least total cost, namely

$$f(x_0) \equiv g(m) = c_0 p^2 \left\{ m-2 + \frac{1}{mp} + 2 \left(\frac{m-1}{m} \cdot \frac{1}{p} - (m-1) \right)^{1/2} \right\} \quad (6)$$

as given by (4).

For case 3 above the decision rests on the question $g(3) \leq g(4)$ and can be settled analytically. The result is that $g(3) < g(4)$.

In the following, we assume case 4, with

$$10 < 1/p \equiv e^X ,$$

the choices being integers $m \geq 2$ for which $m(m+3)/(m-1) < 1/p$, and define M ($M \geq 5$) as the greatest such integer:

$$M(M+3)/(M-1) < 1/p \leq (M+1)(M+4)/M \quad (7)$$

Regarding $g(m)$ as a function of a real variable m on the interval $2 \leq m \leq M$, we find

$$g'(m) = c_0 p^2 \left(1 - \frac{1}{pm^2}\right) \left\{1 - \frac{1}{\sqrt{\frac{m-1}{m} \frac{1}{p} - (m-1)}}\right\} \quad (8)$$

Since $m^2/(m-1)$ is increasing with m for $m \geq 2$ we have

$$m^2/(m-1) \leq M^2/(M-1) < M(M+3)/(M-1) < 1/p, \quad (9)$$

so that the bracket in (8) is positive, and $g'(m)$ has the sign of $s(m) \equiv 1 - \frac{1}{pm^2}$ on $2 \leq m \leq M$

But $s(2) = 1 - \frac{1}{4p} < 0$ since $1/p > 4$, and $s(M) = 1 - \frac{1}{pM^2} > 0$, since by (7),

$1/p < (M+1)(M+4)/M < M^2$ for $M \geq 5$. Hence on the interval $[2, M]$, $g(m)$ is decreasing up to

$$\bar{m} = (1/p)^{1/2} = e^{X/2},$$

is minimal at $\bar{m}$, and increases from $\bar{m}$ to M .

Thus the choice of optimal m lies between the immediately surrounding integers

$$m_1 < (1/p)^{1/2} < m_2 \leq M,$$

depending on the inequality $g(m_1) \leq g(m_2)$. If $(1/p)^{1/2} = \bar{m}$ happens to be an integer, then $\bar{m}$ is of course the cheapest splitting number. In any case, the position of the splitting surface is given by (3), where m is optimal.