A GENERALIZATION OF A CLASSICAL MONTE CARLO ALGORITHM TO ESTIMATE π

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Algoritmul Monte Carlo clasic ***A1*** *estimeazează valoarea numărului* π *bazându-se pe faptul ca raportul dintre aria unui cerc oarecare* C *şi aria pătratului* D *circumscris cercului este egal cu* $\pi / 4$.

Prezentul articol extinde procedura de simulare stocastica ***A1*** *introducând parametrii suplimentari* λ , a , b. *Noul algoritm propus* ***A2***(λ,a,b) *ne conduce la varianta clasică pentru* $\lambda = 0$ *sau* $a.b = 0$.

Variabila aleatoare $W_{\lambda,a,b}$ *ce caracterizează valorile* w *generate de algoritmul* ***A2***(λ,a,b) *constituie un estimator nedeplasat al numărului* π .

În lucrare sunt determinate şi valorile optime λ_* , a_* , b_* *astfel încât variabila aleatoare* $W_{\lambda*,a*,b*}$ *sa aibă cea mai mică dispersie.*

Comparat cu ***A1*** *, precizia estimațiilor furnizate de algoritmul* ***A2***(λ_*,a_*,b_*) *creşte de aproximativ* $\gamma_* = 1.38$ *ori.*

Rezultatele teoretice obținute au fost confirmate practic prin simulare stocastică pe calculator.

It is very known that the ratio between the area of any circle C *and the corresponding area of the circumscribed square domain* D *of* C *is equal to* $\pi/4$. *The classical algorithm* ***A1*** *to estimate the number* π *is based on this remark.*

In the present paper the standard procedure ***A1*** *is extended by considering the additional parameters* λ , a , b . *Our suggested* ***A2***(λ,a,b) *procedure implies the standard variant* ***A1*** *when* $\lambda = 0$ *or* $a.b = 0$.

The random variable $W_{\lambda,a,b}$ *which characterize the outputs* w *of* **A2**(λ,a,b) *algorithm is an unbiased estimator for* π .

More, we determined the optimum values λ_* , a_* , b_* *such that the variance of the random variable* $W_{\lambda*,a*,b*}$ *to attain its minimum value.*

The proposed ***A2***(λ_*,a_*,b_*) *algorithm is approximately* $\gamma_* = 1.38$ *times more accurate than the classical* ***A1*** *Monte Carlo procedure.*

The theoretical results were confirmed experimentally by stochastic simulations on the computer.

Keywords : Estimation of π , Monte Carlo method, stochastic simulation, unbiased estimator, minimum variance.

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Introduction

In the literature there are presented many deterministic and also Monte Carlo algorithms for estimating the unknown value of π (Devroye [2], Dodge [3], Sacuiu, Zorilescu [7]). The classical probabilistic procedures which estimate the number π is based on a rejection type method (Bradley, Fox, Schrage [1], Devroye [2], Gentle [4], Kleijnen [6]).

More precisely, we generate a string of n independent random points $P_i(x,y)$ having an uniform distribution in the square domain $D = \{ (x,y) \mid 0 \le x , y \le 1 \}$. Finally we reject all those points P_i which did not fall inside the circular domain C, $C = \{ (x,y) \mid x \ge 0 , y \ge 0 , x^2 + y^2 \le 1 \}$. Obviously $C \subset D$.

In this manner are retained only m independent random points P_i , with $m \le n$. All these selected points belong to the domain C and are also uniformly distributed on C .

For this reason the number m/n could be considered a good approximation of the ratio $Area(C)/Area(D)$, that is an appropriate estimation for the unknown quantity $\pi/4$.

So, the value of π should be estimated by the quantity $w = 4m/n$.

The classical algorithm ***A1*** determines an estimation w for the number π.

Algorithm *A1*. (The standard rejection procedure for π estimation)

Step 0. Input : the number n of simulation steps.
m = 0 ; j = 0 { j = the current simulation step }

Step 1. j = j + 1
Generate two independent random variates x , y having a uniform U([0 , 1]) distribution

Step 2. (the rejection procedure). If $x^2 + y^2 \le 1$ then $m = m + 1$

Step 3. If $j < n$ then Goto *Step 1*

Step 4. $w = 4m / n$; Print w ; STOP .

In the subsequent we'll generalize the standard algorithm ***A1*** using additional parameters.

Main results

1. A more general algorithm.

Let λ , a , b be fixed real numbers with $a > 0$ and $b > 0$.

We'll define an extension ***A2*** of ***A1*** algorithm by considering the real numbers λ , a , b as additional parameters for ***A2***.

Algorithm *A2*(λ , a , b). (Extension of ***A1*** procedure)

Step 0. Inputs : n (n = the number of simulation steps)

λ , a , b ($\lambda \in \mathbf{R}$, $a > 0$, $b > 0$, $a^2 + b^2 \le 1$)

m = 0 (n = the number of the points P_i which fall in the domain C)

k = 0 (n = the number of the points P_i belonging to [0 , a] x [0 , b] domain)

j = 0 { j = the current simulation step }

Step 1. j = j + 1

Generate two independent random variates x , y having a U([0 , 1]) uniform distribution

Step 2. (the rejection procedure). If $x^2 + y^2 > 1$ then Goto *Step 4*

$m = m + 1$

If $(x \le a) \& (y \le b)$ then k = k + 1

Step 4. If $j < n$ then Goto *Step 1*

Step 5. $w = 4m/n + \lambda k/n - \lambda ab$; Print w ; STOP .

Particular cases :

- Considering $\lambda = 0$ in ***A2*** algorithm we just obtain the classical ***A1*** procedure , ***A2***(0,a,b) ≡ ***A1***.

- At the same conclusion we arrive if we take $ab = 0$ for any $\lambda \in \mathbf{R}$ (***A2***(λ,a,0) ≡ ***A2***(λ,0,b) ≡ ***A1***).

In the following we'll try to prove that for any $\lambda \in \mathbf{R}$ and $a > 0$, $b > 0$ with $a^2 + b^2 \le 1$ the w value produced by ***A2***(λ,a,b) algorithm is an unbiased estimation of π .

More, taking into consideration different variants of ***A2***(λ,a,b) procedure which depend on the parameters λ , a , b we can choose the appropriate values λ_*, a_* , b_* of these parameters such that the estimations w of π to attain a minimum dispersion.

2. Theoretical results.

We define the functions

$$h_1(x,y)=\begin{cases}4 & ; \ \textit{if}\ (x\ge 0, y\ge 0, x^2+y^2\le 1)\\ 0 & ; \ \textit{otherwise}\end{cases} \tag{1}$$

$$h_2(x,y)=\begin{cases}1 & ; \ \textit{if}\ (0\le x\le a, 0\le y\le b)\\ 0 & ; \ \textit{otherwise}\end{cases} \tag{2}$$

In the following we'll impose some restrictions for the unknown values of the parameters a , b . So, we'll consider

Hypothesis H1. $0 \le a , b \le 1$.

Hypothesis H2. $a \ge 0$, $b \ge 0$ and $a^2+b^2\le 1$.

Definition 1. For any independent random variables (r.v.-s) X ,Y which have an uniform distribution on the interval [0 , 1] , X~ U([0 , 1]), Y~ U([0 , 1]) , we define the r.v. $W_{\lambda,a,b}$ given by the expression

$$W_{\lambda,a,b}=h_1(X,Y)+\lambda\left(h_2(X,Y)-ab\right) \tag{3}$$

Remark 1. Analyzing the algorithm ***A2***(λ,a,b) we deduce that its output w can be regarded as an observation from the r.v. $W_{\lambda,a,b}$.

In the subsequent we intend to use the r.v. $W_{\lambda,a,b}$ to study the statistical qualities of the estimations w . More precisely

Proposition 1. For any $\lambda \in \mathbf{R}$ and a , b respecting the restriction **H1** , the r.v. $W_{\lambda,a,b}$ is an unbiased estimation of π , that is

$$Mean(W_{\lambda,a,b})=\pi \tag{4}$$

Proof. The probability density function (p.d.f.) $f_1(x,y)$ of the random vector (X,Y) has the form

$$f_1(x,y)=\begin{cases}1 & ; \ \textit{if}\ (0\le x\le 1, 0\le y\le 1)\\ 0 & ; \ \textit{otherwise}\end{cases}$$

So, we get

$$Mean(W_{\lambda,a,b})=\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\left(h_1(x,y)+\lambda\,(h_2(x,y)-a.b)\right)f_1(x,y)\,dx\,dy=$$

$$=\int_0^1\int_0^1 h_1(x,y)\,dx\,dy+\lambda\int_0^1\int_0^1 (h_2(x,y)-a.b)\,dx\,dy=$$

$$= 4\int_0^1 \left(\int_0^{\sqrt{1-x^2}} dy \right) dx + \lambda \left(\int_0^a \int_0^b dx\, dy - a.b \right) = 4\int_0^1 \sqrt{1-x^2}\, dx =$$

$$= 4\int_0^{\pi/2} cos^2(t)\, dt = 4\int_0^{\pi/2} \frac{1+cos(2t)}{2}\, dt = \pi$$

Proposition 2. If the hypothesis **H2** is satisfied then the variance $Var(W_{\lambda,a,b})$ of the r.v. $W_{\lambda,a,b}$ has the expression

$$Var(W_{\lambda,a,b}) = g_1(\lambda,a,b) = ab(1-ab)\lambda^2 + 2ab(4-\pi)\lambda + \pi(4-\pi) \qquad (5)$$

Proof. Indeed, for any $a \geq 0$, $b \geq 0$ with $a^2 + b^2 \leq 1$ we deduce successively

$$g_1(\lambda,a,b) = Var(W_{\lambda,a,b}) = Mean(W_{\lambda,a,b}^2) - \left(Mean(W_{\lambda,a,b})\right)^2 =$$

$$= \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \left(h_1(x,y) + \lambda\left(h_2(x,y) - a.b\right)\right)^2 f_1(x,y)\, dx\, dy - \pi^2 =$$

$$= \int_0^1\int_0^1 h_1^2(x,y)\, dx\, dy + \lambda^2 \int_0^1\int_0^1 \left(h_2(x,y) - a.b\right)^2 dx\, dy +$$

$$+ 2\lambda \int_0^1\int_0^1 h_1(x,y)\left(h_2(x,y) - a.b\right) dx\, dy - \pi^2 =$$

$$= \int_0^1 \left(\int_0^{\sqrt{1-x^2}} 16\, dy \right) dx + \lambda^2 \int_0^a\int_0^b (1-2ab)\, dx\, dy + \lambda^2 a^2 b^2 +$$

$$+ 2\lambda \int_0^a\int_0^b 4\, dx\, dy - 2\lambda ab \int_0^1 \left(\int_0^{\sqrt{1-x^2}} 4\, dy \right) dx - \pi^2 =$$

$$= 4\pi + \lambda^2 ab(1-ab) + 2\lambda ab(4-\pi) - \pi^2 = ab(1-ab)\lambda^2 + 2ab(4-\pi)\lambda + \pi(4-\pi)$$

Remark 2. The function $g_1(\lambda,a,b)$ defined by the formula (5) is symmetrical one in the arguments a and b , that is $g_1(\lambda,a,b) = g_1(\lambda,b,a)$ for any real values a , b which satisfy the restriction **H2**.

Remark 3. The accuracy of ***A1*** outputs is given by the variance of the r.v. $W_{0,a,b}$ that is $Var(W_{0,a,b}) = \pi(4-\pi) \approx 2.6968$ for any real numbers a, b respecting **H2** hypothesis.

Proposition 3. For given real numbers a , b which verify the restriction **H2** , the minimum value of the variance $Var(W_{\lambda,a,b})$, regarded as a function of λ , is attained for $\lambda = \lambda_1$ where

$$\lambda_1 = \frac{\pi - 4}{1 - ab} \tag{6}$$

and in addition

$$Var(W_{\lambda_1,a,b}) = g_2(a,b) = -\frac{ab}{1-ab}(4-\pi)^2 + \pi(4-\pi) \tag{7}$$

Proof. We'll treat individually the situations $a.b = 0$, respectively $a.b \neq 0$.

Case 1. If $a.b = 0$ then for any $\lambda \in \mathbf{R}$ we have

$$Var(W_{\lambda,a,b}) = g_1(\lambda,a,b) = ab(1-ab)\lambda^2 + 2ab(4-\pi)\lambda + \pi(4-\pi) = \pi(4-\pi)$$

and hence for $\lambda = \lambda_1$ we conclude

$$Var(W_{\lambda_1,a,b}) = \pi(4-\pi) = -\frac{ab}{1-ab}(4-\pi)^2 + \pi(4-\pi) = g_2(a,b)$$

Case 2. Indeed, since $a.b \neq 0$ we deduce that the polynomial function $g_1(\lambda,a,b)$ has the degree two in the variable λ and more it takes its minimum when

$$\lambda = \lambda_1 = -\frac{2ab(4-\pi)}{2ab(1-ab)} = \frac{\pi-4}{1-ab}$$

So, the minimum $g_2(a,b)$ of the function $g_1(\lambda,a,b)$ has the following expression

$$g_2(a,b) = g_1(\lambda_1,a,b) = ab(1-ab)\lambda_1^2 + 2ab(4-\pi)\lambda_1 + \pi(4-\pi) =$$
$$= \pi(4-\pi) - \frac{ab}{1-ab}(4-\pi)^2$$

which finish the proposition proof.

Proposition 4. Respecting the hypothesis **H2**, the minimum variance of the random variables $W_{\lambda,a,b}$ is attained when the parameters a , b , λ take the values

$$a_* = b_* = 1/\sqrt{2} \qquad \lambda_* = 2\pi - 8 \tag{8}$$

and more

$$Var(W_{\lambda_*,a_*,b_*}) = (4-\pi)(2\pi-4) \approx 1.9599 \tag{9}$$

Proof. Taking into consideration the results of Proposition 3 it remains to find those values a_*, b_* which minimize the function $g_2(a,b)$ given by (7).

At the end we'll consider $\lambda_* = (\pi - 4)/(1 - a_* b_*)$.

Case 1. When $a.b = 0$ then the constant function $g_2(a,b) = \pi(4-\pi)$ has obviously its minimum value equal to $\pi(4-\pi)$.

Case 2. Now we'll find the minimum value of the function $g_2(a,b)$ for any $a > 0$, $b > 0$ which respect the inequality $a^2 + b^2 \le 1$.

First, we remark that the function $g_3(t) = t/(1-t)$, $0 < t < 1$, is an increasing one. So, the minimum value for the expression $g_2(a,b)$ given by (7),

$$g_2(a,b) = \pi(4-\pi) - \frac{ab}{1-ab}(4-\pi)^2 = \pi(4-\pi) - \frac{t}{1-t}(4-\pi)^2$$

is obtained when the variable $t = ab$ takes its maximum value, respecting also the restrictions : $a > 0, b > 0, a^2 + b^2 \le 1$.

But the maximum value of $t^2 = a^2 b^2$ with $a^2 + b^2 \le 1$ is attained for $a^2 = b^2 = 1/2$, that is $a_* = b_* = 1/\sqrt{2}$.

Having $a_* = b_* = 1/\sqrt{2}$ we deduce $\lambda_* = (\pi - 4)/(1 - a_* b_*) = 2\pi - 8$.

More

$$Var(W_{\lambda_*, a_*, b_*}) = g_2(a_*, b_*) = \pi(4-\pi) - \frac{a_* b_*}{1 - a_* b_*}(4-\pi)^2 = (4-\pi)(2\pi - 4) = 1.9599$$

Analyzing both previous alternatives, since $(4-\pi)(2\pi-4) < (4-\pi)\pi$ we deduce the results mentioned by Proposition 4.

3. A Monte Carlo study.

Figure 1 presents the graphic of the function $g_2(a,a) = Var(W_{\lambda_1,a,a})$ which has the form (7). We mention here that $g_2(a,a)$ is a decreasing application.

Comparing with ***A1***, the algorithm ***A2***(λ_1,a,b) is $\gamma(a,b)$ times more accurate to estimate π. The coefficient $\gamma(a,b)$ is just the ratio

$$\gamma(a,b) = \frac{Var(W_{0,a,b})}{Var(W_{\lambda_1,a,b})} = \frac{\pi(4-\pi)}{g_2(a,b)} = \frac{\pi}{\pi - ab(4-\pi)/(1-ab)} \qquad (10)$$

Obviously $\gamma(a,b) = \gamma(b,a)$.

Table 1 lists the values of $\gamma(a,a)$ when $0 \le a \le 1/\sqrt{2}$.

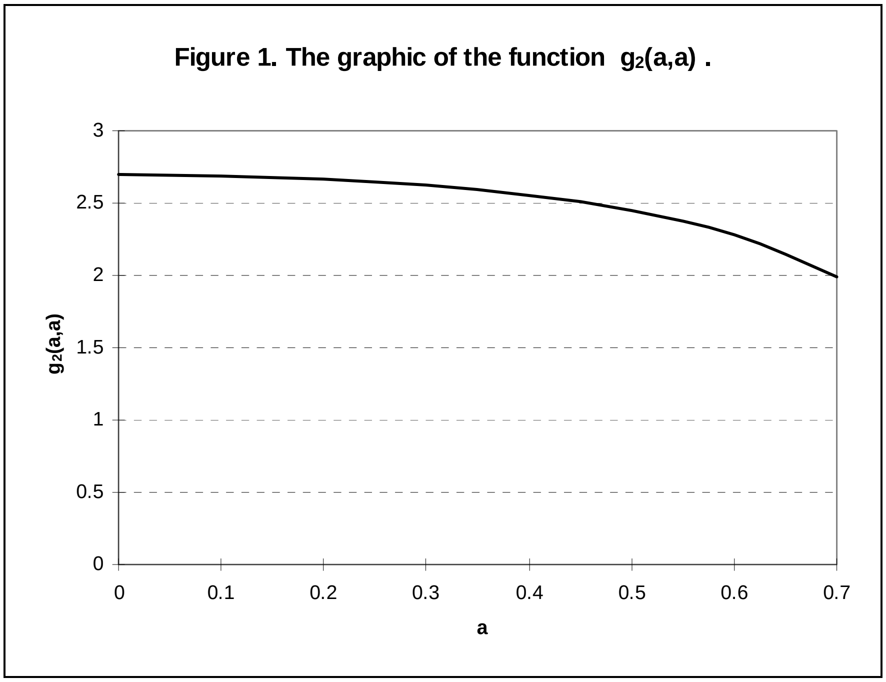

Table 1

The values of the coefficient $\gamma(a,a)$.

a	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7
γ(a,a)	1.000	1.003	1.012	1.028	1.055	1.100	1.182	1.356

The maximum value γ_* of the indicator $\gamma(a,b)$ is attained for $a_* = 1/\sqrt{2}$ and $b_* = 1/\sqrt{2}$, that is

$$\gamma_* = \frac{Var(W_{0,a_*,a_*})}{Var(W_{\lambda_*,a_*,a_*})} = \frac{\pi(4-\pi)}{(2\pi-4)(4-\pi)} = \frac{\pi}{2\pi-4} = 1.376 \qquad (11)$$

Table 2 gives the optimum values λ_1 computed with formula (6) for the parameter λ of ***A2***(λ,a,a) algorithm (the case $a = b$).

Table 2

The optimum value λ_1 (formula (6), the case a = b).

a = b	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7
λ_1	0.0000	-0.8687	-0.8958	-0.9450	-1.0238	-1.1467	-1.3438	-1.6863

Running the algorithm ***A2***(λ_1,a,a) for n=1000 we obtained the estimations w of π , quantities which are listed in Table 3. This process was repeated s = 20 times, the variable s counting the current simulated step.

Table 3

The outputs w of *A2*(λ_1,a,a) algorithm (n=1000 , s=20 simulations).

s	a = 0.0	a = 0.1	a = 0.2	a = 0.3	a = 0.4	a = 0.5	a = 0.6	a = 0.7
1	3.156	3.153	3.153	3.163	3.149	3.138	3.136	3.124
2	3.052	3.054	3.052	3.053	3.054	3.051	3.076	3.064
3	3.056	3.058	3.055	3.062	3.058	3.062	3.075	3.044
4	3.148	3.150	3.147	3.151	3.138	3.155	3.169	3.188
5	3.084	3.081	3.075	3.075	3.083	3.095	3.095	3.108
6	3.144	3.143	3.139	3.133	3.141	3.151	3.140	3.142
7	3.196	3.198	3.203	3.202	3.188	3.190	3.183	3.179
8	3.200	3.196	3.199	3.191	3.195	3.193	3.208	3.192
9	3.160	3.161	3.158	3.156	3.153	3.151	3.148	3.120
10	3.184	3.187	3.180	3.178	3.179	3.163	3.164	3.165
11	3.128	3.126	3.125	3.126	3.126	3.121	3.143	3.130
12	3.184	3.186	3.184	3.177	3.166	3.167	3.149	3.122
13	3.232	3.228	3.220	3.223	3.223	3.216	3.225	3.188
14	3.104	3.102	3.098	3.099	3.098	3.095	3.088	3.082
15	3.136	3.139	3.138	3.139	3.146	3.155	3.145	3.129
16	3.072	3.069	3.079	3.082	3.070	3.058	3.077	3.084
17	3.232	3.227	3.237	3.232	3.227	3.234	3.210	3.215
18	3.204	3.203	3.198	3.197	3.192	3.176	3.162	3.155
19	3.008	3.009	3.012	3.012	3.023	3.034	3.050	3.050
20	3.088	3.089	3.088	3.087	3.099	3.106	3.107	3.122

Taking into consideration the outputs w_k , $1 \le k \le s$, produced after s independent runs of ***A2***(λ_1,a,a) procedure we are also computed the mean μ and the dispersion σ^2 of these experimental results, where

$$\mu = \frac{w_1 + w_2 + w_3 + \ldots + w_s}{s}$$

$$\sigma^2 = \frac{(w_1 - \mu)^2 + (w_2 - \mu)^2 + (w_3 - \mu)^2 + \ldots + (w_s - \mu)^2}{s} \tag{12}$$

The values of μ and σ^2 indicators obtained for different values for the input parameter a of ***A2***(λ_1,a,a) estimation procedure are presented in Table 4.

The experimental data confirm the theoretical results. More precisely, the dispersion σ^2 decreases when the values of the parameter a increase (compare Figure 1 with Table 4).

Table 4

The mean μ and the variance σ^2 for the outputs w of $A2(\lambda_1$,a,a) algorithm considering s=20 simulation runs (n=1000).

	a = 0.0	a = 0.1	a = 0.2	a = 0.3	a = 0.4	a = 0.5	a = 0.6	a = 0.7
μ	3.138	3.138	3.137	3.137	3.135	3.136	3.138	3.130
σ^2	0.00382	0.00374	0.00373	0.00355	0.00321	0.00302	0.00234	0.00228

Concluding remarks

Imagining new parameters to the classical ***A1*** estimation algorithm we obtained the extended procedure ***A2***(λ,a,b). The procedure ***A1*** is deduced from ***A2***(λ,a,b) as a particular case, that is by considering $\lambda = 0$ or $ab = 0$ (***A2***(0,a,b) ≡ ≡ ***A2***(λ,a,0) ≡ ***A2***(λ,0,b) ≡ ***A1***).

A theoretical proof (Proposition 1) confirms the good properties of w outputs produced by ***A2***(λ,a,b) procedure to evaluate the unknown value of π (the random variable $W_{\lambda,a,b}$ is an unbiased estimator for π). The dispersion of the estimator $W_{\lambda,a,b}$ is also computed (see Proposition 2).

More, we determined the optimum values λ_* , a_* , b_* for the parameters of ***A2***(λ,a,b) generalized algorithm such that the outputs w to have a minimum dispersion (Proposition 4).

A Monte Carlo computer simulation confirmed the theoretical results (see Table 4).

In conclusion, the suggested ***A2***(λ_*,a_*,b_*) algorithm is approximately γ_* = 1.376 times more accurate than the standard ***A1*** Monte Carlo procedure.

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