MONTE CARLO METHOD APPLIED TO THE SOLUTION OF SIMULTANEOUS LINEAR EQUATIONS

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1. Introduction

The matrix inversion by Monte Carlo method is deviced originally by J. von Neumann and S. M. Ulam and developed by G. E. Forsythe and R. A. Leibler [1], [2], [3]. In this paper we shall present an application of the so-called "splitting technique" to the matrix inversion by Monte Carlo method [4]. The mean number of random digits required for one particle history and its variance are also given. The more general results about the splitting technique will be presented in the forthcomming paper.

2. Transformation of simultaneous linear equation

In this section we shall show the following :

LEMMA.

Every simultaneous linear equation can be reduced to the form

$$(I-S)x=c$$

where S is a positive definite matrix with the largest eigenvalue less than 1 and with $M\equiv\max_i\sum_j|s_{ij}|$ less than 2, and x, c denote unknown and known vectors, respectively.

PROOF. Given a simultaneous linear equation

$$Az=b$$

we can transform it into the form

$$A'Az=A'b$$

where A' denotes the transposed matrix of A.
Denoting $B\equiv A'A$, $\delta=A'b$, we have

$$Bz=\delta$$

with positive definite B. Then there exist matrices U and $\begin{pmatrix}\sqrt{b_{11}} & & 0\\ & \ddots & \\ 0 & & \sqrt{b_{nn}}\end{pmatrix}$

such that $B=\begin{pmatrix} \sqrt{b_{11}} & & 0 \\ & \ddots & \\ 0 & & \sqrt{b_{nn}} \end{pmatrix} U \begin{pmatrix} \sqrt{b_{11}} & & 0 \\ & \ddots & \\ 0 & & \sqrt{b_{nn}} \end{pmatrix}$. Thus we obtain

$$\begin{pmatrix} \sqrt{b_{11}} & & 0 \\ & \ddots & \\ 0 & & \sqrt{b_{nn}} \end{pmatrix} U \begin{pmatrix} \sqrt{b_{11}} & & 0 \\ & \ddots & \\ 0 & & \sqrt{b_{nn}} \end{pmatrix} z=\delta$$

or

$$Ux=\delta^*$$

where $x=\begin{pmatrix} \sqrt{b_{11}} & & 0 \\ & \ddots & \\ 0 & & \sqrt{b_{nn}} \end{pmatrix} z$, $\delta^*=\begin{pmatrix} \frac{1}{\sqrt{b_{11}}} & & 0 \\ & \ddots & \\ 0 & & \frac{1}{\sqrt{b_{nn}}} \end{pmatrix} \delta$ and $u_{ii}=1$. Putting $\tau=$ $\min(n, \sqrt{n}M)$ we have $Rx=c$ where $R=\tau^{-1}Uc$ $=\tau^{-1}\delta^*$. R is positive definite and its maximum eigenvalue is less than 1.

When we put $S=I-R$, we obtain the desired result.

3. Process of operation

According to the preceding lemma we shall in the following concern ourselves with the case where the maximum eigenvalue of $|S|\equiv(|s_{ij}|)$ is less than 1. In this section we want to obtain an estimate of $(I-S)^{-1}$ $\equiv(\beta_{ij})$. For that purpose we take

$$P=\begin{array}{c} \overset{\longleftarrow k \longrightarrow \longleftarrow k \longrightarrow}{\begin{pmatrix} P_{11} & Q \\ O & I \end{pmatrix}} \begin{array}{l} \updownarrow k \\ \updownarrow k \end{array} \end{array}$$

as our transient probability matrix where

$$P_{11}=(p_{ij}) \quad p_{ij}=\frac{|s_{ij}|}{\sigma}; \ \sigma=2 \text{ for } M\geq 1$$

$$\sigma=1 \text{ for } M<1$$

$$Q=(\delta_{ij}q_j) \quad q_j=1-\sum_{k=1}^{k} p_{jk}\,.$$

Now, consider a particle with weight 1 at i and take a random number to decide whether the particle should go to some $j(=1, 2, \cdots, k)$ with probability p_{ij} or should be trapped at i with probability q_i. When the particle is transmitted to j from i we split it into σ new independent particles multiplied by the weighting factor sgn s_{ij}. We thus accumulate the total weight of particles trapped at j from a particle which started from i, and represent it as $X(ij)$. We then take $b_{ij}=\frac{X(ij)}{q_j}$ as an estimate of β_{ij}.

4. Properties of b_{ij}

We shall represent the total weight of particles which have been trapped at j from a particle which have started from i up to the n-th generation by $X_n(ij)$, and $\frac{X_n(ij)}{q_j}$ by b_{ij}^n. As will be shown in section 6, the mean number of random digits required for obtaining $X(ij)$ is finite, so it can be seen that $X_n(ij)$ and b_{ij}^n tend in probability to $X(ij)$ and b_{ij}, respectively. Thus we have :

LEMMA.

$$\begin{aligned} X_n(ij) &\to X(ij) \\ b_{ij}^n &\to b_{ij} \end{aligned} \qquad \text{i.p.} \quad (n\to+\infty)$$

We then have the following theorems about the mean and variance of $X(ij)$ and b_{ij}.

THEOREM 1.

$$(Eb_{ij})=(I-S)^{-1}. \quad (EX(ij))=(I-S)^{-1}Q.$$

PROOF. We can easily get the following recurrence relation.

$$\begin{aligned} E(X_{n+1}(ij)) &= \delta_{ij}q_j+\sum_{i_1=1}^{k}p_{ii_1}(\operatorname{sgn} s_{ii_1})\sigma E(X_n(ij)) \\ &= \delta_{ij}q_j+\sum_{i_1=1}^{k}s_{ii_1}E(X_n(ij)) \\ E(X_1(ij)) &= \delta_{ij}q_j . \end{aligned}$$

Thus we have

$$(E(X_n(ij)))=(I+S+\cdots+S^{n-1})Q$$

and

$$(Eb_{ij}^n)=(I+S+\cdots+S^{n-1}).$$

By making n infinitely large, we get the wanted results.

THEOREM 2.

$$(D^2X(ij))=(I-|S|)^{-1}(Q+(\sigma|S|-I)(E^2))$$

where $(E^2)=(E^2X(ij))$.

PROOF. It holds that

$$\begin{aligned}EX_{n+1}^2(ij)&=\delta_{ij}q_j+\sum_{i_1=1}^{k}p_{ii_1}E(X_n(i_1j)(\omega_1)+\cdots+X_n(i_1j)(\omega_\sigma))^2\\&=\delta_{ij}q_j+\sum_{i_1=1}^{k}p_{ii_1}\sigma EX_n^2(i_1j)+\sum_{i_1=1}^{k}p_{ii_1}\sigma(\sigma-1)E^2X_n(i_1j)\\&=\delta_{ij}q_j+\sum_{i_1=1}^{k}|s_{ii_1}|EX_n^2(i_1j)+(\sigma-1)\sum_{i_1=1}^{k}|s_{ii_1}|E^2X_n(i_1j)\,.\end{aligned}$$

Thus we get

$$\begin{aligned}(EX_{n+1}^2(ij))&=(I+|S|+\cdots+|S|^n)Q\\&\quad+(\sigma-1)|S|((E_n^2)+|S|(E_{n-1}^2)+\cdots+|S|^{n-1}(E_1^2))\,.\end{aligned}$$

When n tends to infinity, we have

$$\begin{aligned}(EX^2(ij))&=(I-|S|)^{-1}Q+(\sigma-1)(I-|S|)^{-1}|S|(E^2)\\&=(I-|S|)^{-1}(Q+(\sigma-1)|S|(E^2))\,.\end{aligned}$$

Remark: Proofs of the above two theorems show that as σ we can take any integral value for which $M/\sigma<1$ holds. But the above proof shows that the smaller the σ the smaller the $D^2X(ij)$. This is the reason why we take σ as defined before. But our method is not necessarily an effective one. For example, we have an effective one when we apply our splitting technique only for transmission from i to j corresponding to large $|s_{ij}|$ instead of using one and the same factor σ for all $|s_{ij}|$. We take the above procedure only for its simplicity of operation.

5. Effectiveness of splitting technique

When we adopt the ordinary weighting process described in the paper of Forsythe and Leibler using our P, we have only to multiply the particle by the weighting factor $\sigma\,\mathrm{sgn}\,s_{ij}$ in case it goes from i to j. In this case

$$(EX_{n+1}^2(ij))=Q+\sigma|S|(EX_n^2(ij))\,,$$

and we can not have finite $(D^2X(ij))$ so long as the maximum eigenvalue of $|S|$ is not less than $1/\sigma$. Actually we have an example of S with maximum eigenvalue less than 1, $M>1$ and with maximum eigenvalue of $|S|$ lying between 0.5 and 1.

6. Mean and variance of the number of random digits required for one particle history

By $W_n(i)$ we shall represent the total number of random digits required or obtaining the n-th generation of a particle starting from i.

Then we have the following:

THEOREM 3.

$$(EW_{n+1}(i))=|S|(EW_n(i))+e$$

$$(EW_1(i))=e$$

$$(D^2W_{n+1}(i))=|S|(D^2W_n(i))+\sigma|S|(E^2W_n(i))$$
$$+2|S|(EW_n(i))+e-(E^2W_n(i))$$

$$(D^2W_1(i))=O$$

where $e=(1, 1, \cdots 1)'$ $O=(0, 0, \cdots 0)'$.

PROOF. As in the proofs of the former theorems, we have

$$EW_{n+1}(i)=1+\sum_{j=1}^{k}p_{ij}\sigma EW_n(j)=1+\sum_{j=1}^{k}|s_{ij}|EW_n(j)$$

$$EW_{n+1}^2(i)=\underset{\omega,j}{E}(1+W_n(j)(\omega_1)+\cdots+W_n(j)(\omega_\sigma))^2$$

$$=1+2\sum_{j=1}^{k}p_{ij}\sigma EW_n(j)+(\sigma-1)\sum_{j=1}^{k}p_{ij}\sigma E^2W_n(j)$$

$$+\sum_{j=1}^{k}p_{ij}\sigma EW_n^2(j)\,.$$

The above proof shows that

$$(EW_{n+1}(i))=(I+|S|+\cdots+|S|^n)e\leq(I-|S|)^{-1}e\,.$$

It can be seen by this inequality that the probability that a particle eventually dies is equal to unity. This facts assures us the validity of our lemma in section 4. We have the following:

THEOREM 4. *When we represent the total number of random digits required for obtaining a whole history of a particle which started form i by $W(i)$, we have*

$$(EW(i))=(I-|S|)^{-1}e$$

$$(D^2W(i))=(I-|S|)^{-1}(2|S|(EW(i))+e+(\sigma|S|-I)(E^2W(i)))\,.$$

7. Computing procedure for splitting technique

Consider now a computing layout:

Number of Generation	0	1	2	3	4
+	[i]	$\times$			
$-$					
+	[i]				
$-$		(i_1)	$\times$		
+		$\downarrow$	(i_2)	$\times$	
$-$		[i_1]	$\downarrow$		
+			[i_2]	$\times$	
$-$					

0. We start a particle from i. We write [i] in the + row of the 0-th generation column. Take a random digit and transmit the particle according to P.

1. If it is trapped at i, write $\times$ right to the [i] and stop the operation.

2. If it is transmitted to $i_1(=1, 2, \cdots k)$, write i_1 on the 1st generation column in the same row of [i] in case $\operatorname{sgn} s_{ii_1}=1$ and in the opposite row in case $\operatorname{sgn} s_{ii_1}=-1$.

3. Take the next random digit.

4. If a particle is trapped at i_1, write $\times$ right to the i_1 in the 2nd generation column. When $\sigma=2$, then parenthesize the i_1 and start another new particle from [i_1].

5. If particle is transmitted to i_2, write i_2 in the 2nd generation column on the same row of i_1 in case $\operatorname{sgn} s_{i_1 i_2}=1$ and on the opposite row in case $\operatorname{sgn} s_{i_1 i_2}=-1$.

6. Continue the process until there is no i_ν left without ( ).

7. Repeat the same process for N new particles.

8. Count the js just left to the $\times$ with their signs suggested by their position on the row, and get $\sum_{\nu=1}^{N} X(ij)(\omega_\nu)$.

8. Concluding remarks

Process adopted in this paper is one of the simplest type of branching or multiplicative process and every results are also directly obtainable from the general theory [5] [6]. We are preparing to put these process on the FACOM-118 automatic relay computer. Experimental results will be presented in some future occasion.

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