On Linear Equations and Markov Chains

Application of the Monte Carlo method
in the simulation of stochastic processes

Linear Equations: In general Markov Chain Monte Carlo (*MCMC*) methods to solve *n* by *n* systems of linear equations **Bx = f** are not competitive with classical numerical methods. Still, there are some situations where the *MCMC* methods can be successfully used:

- The size of matrix **B** is very large ($n > 10^3$) and a rough estimate of **x** is required.
- When we are interested to estimate onlya few of the elements of **x.**

Here we follow Rubinstein [7]. Let us consider a system of simultaneous linear equations written in matrix form

$$\mathbf{B}\,\mathbf{x} = \mathbf{f}\,. \tag{1}$$

where the column vector **x** is to be found and the square matrix $B = \left\| b_{ij} \right\|_1^n$ and the column vector **f** are given. Introducing **B = I-A**, where **I** is an identity matrix, system (1) can be written as

$$\mathbf{x} = \mathbf{A}\,\mathbf{x} + \mathbf{f}\,. \tag{2}$$

Suppose $\max_i \sum_{j=1}^{n} \left| a_{ij} \right| < 1;\ i = 1, 2, ..., n\,.$ (3)

Under this assumption we can solve (2) by applying the following recursive equation:

$$\mathbf{x}^{(k+1)} = \mathbf{A}\mathbf{x}^{(k)} + \mathbf{f}\,. \tag{4}$$

Assuming $\mathbf{x}^0 \equiv \mathbf{0}$ and $\mathbf{A}^0 \equiv \mathbf{I}$, we have

$$\mathbf{x}^{(k+1)} = (\mathbf{I} + \mathbf{A} + ... + \mathbf{A}^{k-1} + \mathbf{A}^k)\,\mathbf{f} = \sum_{m=0}^{k} \mathbf{A}^m\,\mathbf{f}\,.$$

Taking the limit, for **B** nonsingular,

$$\lim_{k \to \infty} \mathbf{x}^{(k)} = \lim_{k \to \infty} \sum_{m=0}^{k} \mathbf{A}^m\,\mathbf{f} = (\mathbf{I} - \mathbf{A})^{-1}\,\mathbf{f} = \mathbf{B}^{-1}\,\mathbf{f} = \mathbf{x}\,, \tag{5}$$

we obtain the exact solution of **x**.

As we can see from the text above Rubinstein [7] – in order to find the exact solution **x –** is assuming (3) is true and **B** is nonsingular. We are now going to show that if condition (3) is true then **B** is nonsingular. This means that *MCMC* methods for solving systems of linear equations never fail because of condition (3). On the other hand in general we can use condition (3) as a test for the singularity of square matrix **B**.

Theorem 1: Let **B = I-A**, where **I** is an identity matrix, $\mathbf{B} = \left\| b_{ij} \right\|_1^n$ and $\mathbf{A} = \left\| a_{ij} \right\|_1^n$ are square matrices. If

$$\max_i \sum_{j=1}^{n} \left| a_{ij} \right| < 1\,,\ i = 1, 2, ...\ n, \tag{6}$$

where | | denotes the absolute value, then *det* **B** > 0 and matrix **B** is nonsingular.

Proof:

$$det\,\mathbf{B} = (1 - a_{nn})\,det B_{nn} - \sum_{j=1}^{n-1} (-1)^{n+j} a_{nj}\,det\,B_{nj}\,, \tag{7}$$

where B_{nj}, $j = 1, \ldots, n$ are *minors* of matrix **B.**
It can be easily shown that

$$\frac{\left| det\,B_{nj} \right|}{\left| det\,B_{nn} \right|} < 1. \tag{8}$$

Now we can rewrite (7) in this form

$$\frac{1}{det\,B_{nn}}\,det\,B = 1 - a_{nn} - \sum_{j=1}^{n} (-1)^{n+j}\,a_{nj}\,\frac{det\,B_{nj}}{det\,B_{nn}}\,. \tag{9}$$

From (6), (8) and (9) finally follows that

$det\,\mathbf{B} > 0\,.$ *Q.E.D.*

By using the Monte Carlo method we can explore the set over which the theorem is to be tested in an efficient manner:

Algorithm 1:
Input: *N* **-** number of random numbers with uniform distribution *U*(0,1), *n* - dimension of matrix **B**.
Output: message "*det* **B** ≤ 0".

```
For k = 1 to N
   For i,j =1 to n
       aij ← U(0,1)
       sgn ← U(0,1)
       if (sgn < 0.5) then
              aij = - aij
       endif
   next i,j
   if (max_i Σ_{j=1}^{n} |aij| < 1) then
       if (det B ≤ 0) then
              message "det B ≤ 0"
       endif
   endif
next k
```

The theorem has been tested for *N* = 1000000 and *n* = 3. The message "*det* **B** ≤ 0" never appeared.

References

1. Fishman, G. S.: Monte Carlo: concepts, algorithms, and applications. Springer, 1996.
2. Hammersley, J. M. and Handscomb, D. C.: Monte Carlo Methods. Chapman and Hall, 1964.
3. Knuth, D.: The Art of Computer Programming: Semi-numerical Algorithms. Vol.2 , 2nd ed., Addison-Wesley, 1981.
4. Pllana, S.: Primjena metode Monte Carlo u simulaciji stohastickih procesa s pomocu racunala: Magistarski rad. FER Sveuciliste Zagreb, 1997.
5. Press, W. H. and Teukolsky S. A. and Vetterling W. T. and Flannery B. P.: Numerical Recipes in FORTRAN: The Art of Scientific Computing. Cambridge University Press, 1994.
6. Ripley, B. D.: Stochastic Simulation. John Wiley & Sons, Inc., 1987.
7. Rubinstein, R. Y.: Simulation and the Monte Carlo method. John Wiley & Sons, Inc., 1981.
8. Tanner, M. A.: Tools for statistical inference: methods for the exploration of posterior distributions and likelihood functions. Springer, 1996.

Sabri Pllana, Klancic 4, 51521 Punat, Croatia, Tel. & Fax: +385-1-660 2670, WWW: http://www.geocities.com/CollegePark/Quad/2435/, email: sabri@pinus.cc.fer.hr