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How to Transform B-Matrix Chains into Markov Chains and Vice Versa

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Abstract:- The two basic hypotheses of Markov chains and the four basic hypotheses of B-Matrix chains proposed are carefully examined and compared to find a way to improve Markov chainsin certain specific situations . Our objective is to allow Markov chains to handle boundary conditions and / orsource / sink term in addition to ensuring the stability and convergence of the Markov series.

Moreover, the numerical analysis of the eigenvalues of the proposed matrix B and of its eigenvectors validates the proposed following principle: [For positive symmetric physical power matrices, the sum of their eigenvalues is equal to the eigenvalue of their sum of power series]. This principle facilitates the search for summation solutions of many infinite algebraic power series such as [(1 + x) / 2] ^ N. We therefore recommend the proposed improvement which is promising in many areas.

I. INTRODUCTION

A Markov chain is a mathematical system that undergoes consecutive transitions from one state to another according to certain probabilistic rules defined in the stochastic Markov matrix itself.

The prominent defining characteristic of the first order Markov chain is that it is memoryless in the sense that it doesn't matter how the process got to its current state. The possible future states are fixed and depend only on the present.

In fact, the characteristic matrix of the original Markov chain M, introduced in 1906, resides only on two axioms, namely that all Mi,j are elements of [0,1] and that the sum of Mi,j over any row (or column) is equal to 1.

The M chains can be applied to find the temporal evolution of the states of an isolated system as a function of its initial conditions IC called the initial state vector U (0) but implicitly without borders or source / sink terms present.

It states that:
at time t = N d t where d t is the time interval for a time jump or a step, U (t) symbolized by U ^ N is given by, [1]
U^N (t)= M^ N U(0). . . . . (1)
N=1,2, ..., infinite large number.

Since the principal eigenvalue of M is 1, it follows that the principal eigenvalue for all Markov power matrices, M ^ 2, M ^ 3, .. M ^ N matrices is unity for all N. This property preserves the conservation of the vector concerned as a solution of a scalar function, that is to say total number of objects, total energy. . .etc.

However, since then two main improvements, namely the symmetry of M and the constancy of its main diagonal entries, have been tested, creating particular M-stochastic matrix chains based on 4 axioms instead of 2.

The proposed B-stochastic transition matrix and its chains follow exactly the same concept of modified Markov chains, but the structure of the B-matrix is greatly improved due to an inherent essential condition or axiom comprising the boundary conditions and the source terms.

In fact, this can be seen as an improvement over conventional Markov applications.

This results in a spatio-temporal solution of the B-chains to the problem IC-BC is given by equation (2). [2.3]

U(x, t) ^{N} = D (b + S) + B ^ N . U (x,0). . . . . (2)
where,
b is the vector BC.
S is the source / sink term.
D is the transfer matrix and is defined by equality,
D = E-I. . . . . (3)
while the matrix E itself is given by,
E = B ^ 0 + B + B ^ 2 +. . . . . . + B ^ N.. . . . (4) [2,3]
Obviously, B ^ 0 = I

It is clear that while N goes to infinity, B ^ N tends towards the null matrix, because one or more summations of B rows are defined to be less than 1. This is a necessary condition for the convergence of equation (4) which is added to matrix B.
Consequently, the eigenvalues of the matrix D are less than unity to allow the contribution of BC.

For sufficiently large N, the power series of matrix B, Equation (4) can be identified equivalent to:

$E = (I-B)^{\wedge -1}$.. .... (5)

It is clear that Eq.2 which has been successfully applied to solve the Laplace and Poisson PDE [2,3] is more general than Markov Equation (1).

Now, the question is whether we can implement the added conditions of matrix B in Markov chains characterized by matrix M, even partially, to approach the chains of matrix B in order to allow considering BC or S ?

This makes the subject of the present article.

II. THEORY

An original Markov process is described by a square matrix M (nxn) whose inputs $M_{i,j}$ satisfy the following two conditions: [1]

i- All inputs $M_{i,j}$ are real and element of the closed interval [0,1]
ii-The sum of the entries for all columns (or all rows) is equal to 1.

However, since Markov's time, many attempts to improve M have been made by adding one or two other conditions, for example,

iii- $B_{i,i}$ = RO = 0 for all i = 1,2, ... n, which means that the main diagonal consists of constant entries RO = 0 that is to say that M is a null principal diagonal matrix which corresponds to the assumption of a null residue after each step of time dt for all the free nodes. Consequently, several tests have been performed recently to improve Markov chains by implementing condition (iii) but only limited to RO = 0 which is a special case of RO element of [0,1] in the case of B-matrix.

As an example, a simple model is formulated by de Jong et al [4] to describe the behavior of first order modified Markov chains in which transitions from one state to itself are excluded. This attempt is actually a special case of B-chains, when the diagonal input RO is assumed to be zero.

However, condition (iii) turned out to be interesting and suitable for research on chemical and biochemical reactions.
iv- $M_{i,j} = M_{j,i}$

which means that the stochastic transition matrix M (i, j) is assumed symmetric.

In this article, the proposed transition matrix B follows the 4 conditions above, but in addition, it complements them with two important innovations:

a-RO is not necessarily zero but can take any value in the closed interval [0,1].

It follows that $B_{i,j}$ = 1/4-RO / 4 for 2D and 1/6-RO / 6 ,for i, j adjacent in 2D and 3D configuration respectively and $B_{i,j}$ = 0 otherwise.

b- The sum of the entries of all the rows adjacent to the limits is less than 1 and far from the limits this sum is equal to the unit.

Condition b allows a space to take into account the value of the boundary conditions BC as well as the source / sink term.

Far from the boundaries, and when the symmetry condition applies, the transition matrix B transforms into a doubly stochastic transition matrix superior than the original Markov matrix which is only a single stochastic transition matrix.

Consequently, the matrix B is uniquely defined by the above conditions i to iv and can be constructed simply for 2D and 3D configurations as indicated later in section III-Applications. In addition, these conditions allow the B-Matrix chains to simultaneously process BC and IC with the term source / sink S in the heat diffusion PDE. [5] Here we summarize the most important contribution that leads to many advantages for B chains over Markov chains:

i-Markov chains may converge towards the required solution and may not, an additional condition is required while the convergence of all the B-chains towards the solution of the IC-BC problem is ensured for all the values of RO element of [0.1].

ii- It is not easy to find eigenvalues and eigenvectors for M-Matrix while it is simple for B-Matrix and for its summation of the power series E or D.

III-Markov chains are not able to process S or BC, but B chains can.
However, in order not to worry too much about the details of the theory, let's move on to the following illustrative applications:

III. APPLICATIONS

III. A-2D Configuration.

Figure 1 shows 9 free nodes, with 12 BC, equally spaced in a 2D rectangular configuration.

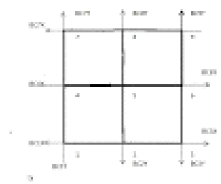

Fig. 1- 9 free nodes, with 12 BC, equally spaced in a 2D rectangular configuration.

The 2D, 9 free nodes of figure 1 are processed by the B-chains as follows : [2,3,5]

First, the matrix inputs $M_{i,j}$ 9x9 are constructed according to Fig.1 and the statistical basis described by conditions i-iv, namely

B=
1-RO 1/4-RO/4 0.0000 1/4-RO/4 0.0000 0.0000 0.0000 0.0000 0.0000

2- 1/4-RO/4 RO 1/4-RO/4 0.0000 1/4-RO/4 .0000 0.0000 0.0000 0.0000

3- 0.00000 1/4-RO/4 RO 0.0000 0.0000 1/4-RO/4 0.0000 0.0000 0.0000

4- 1/4-RO/4 0.0000 0.0000 RO 1/4-RO/4 0.0000 1/4-RO/4 0.0000 0.0000

5- 0.0000 1/4-RO/4 0.0000 1/4-RO/4 RO 1/4-RO/4 0.0000 1/4-RO/4 0.0000

6-0.0000 0.0000 1/4-RO/4 0.0000 1/4-RO/4 RO 0.0000 0.0000 1/4-RO/4

7-0.000 0.0000 0.0000 1/4-RO/4 0.0000 0.0000 RO 1/4-RO/4 0.0000

8- 0.0000 0.0000 0.0000 0.0000 1/4-RO/4 0.0000 0.1500 RO 1/4-RO/4

9- 0.0000 0.0000 0.0000 0.0000 0.0000 1/4-RO/4 0.0000 1/4-RO/4 RO

For example, if we arbitrarily choose the main input of the diagonal constant RO = 0.4, not necessarily zero, then the matrix B reduces to:
1 to 0.400 0.1500 0.0000 0.1500 0.0000 0.0000 0.0000 0.0000 0.0000

2- 0.1500 0.400 0.1500 0.0000 0.1500 .0000 0.0000 0.0000 0.0000

3- 0.00000 0.1500 0.400 0.0000 0.0000 0.1500 0.0000 0.0000 0.0000

4- 0.1500 0.0000 0.0000 0.400 0.1500 0.0000 0.1500 0.0000 0.0000

5- 0.0000 0.1500 0.0000 0.1500 0.400 0.1500 0.0000 0.1500 0.0000

6-0.0000 0.0000 0.1500 0.0000 0.1500 0.400 0.0000 0.0000 0.1500

7-0.000 0.0000 0.0000 0.1500 0.0000 0.0000 0.400 0.1500 0.0000

8- 0.0000 0.0000 0.0000 0.0000 0.1500 0.0000 0.1500 0.400 0.1500

9- 0.0000 0.0000 0.0000 0.0000 0.0000 0.1500 0.0000 0.1500 0.400

For N sufficiently large The matrix B ^ N converges to zero for any value of RO of element of [0,1 [and converges to one for RO = 1

It follows that, only if the BCs are all zeros, then the steady-state equilibrium solution for any initial state is assumed to be the zero vector.

In order for matrix B above to be transformed into an M-Matrix, all of its rows except row 5 must be replaced with the sum 1.

On the other hand, a 9x9 matrix M with all its row summations equal to unity, one or more of its row summations must be modified to make a sum less than 1.

III.B-3 D CONFIGURATION.

Figure 2 shows the simplest 3D configuration, a cube with 8 free nodes and 24 BC

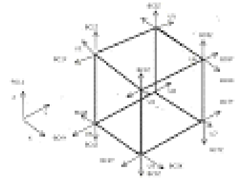

Fig.2 a cube of 8 free nodes and 24 BC [ref 2]

The entries of the matrix $M_{i,j}$ are constructed according to Fig.2 plus a statistical basis described by the conditions i-iv, namely,
B=
1- RO 1/6-RO/6 1/6-RO/6 0,0000 1/6-RO/6 0,0000 0,0000 0,0000
2- 1/6-RO/6 RO 0.0000 1/6-RO/6 0.0000 1/6-RO/6 0.0000 0.0000
3- 1/6-RO/6 0.0000 RO 1/6-RO/6 0.0000 0.0000 1/6-RO/6 0.0000
4- 0.0000 1/6-RO/6 1/6-RO/6 RO 0.0000 0.0000 0.0000 1/6-RO/6
5- 1/6-RO/6 0.0000 0.0000 0.0000 RO 1/6-RO/6 1/6-RO/6 0.0000
6- 0.0000 1/6-RO/6 0.0000 0.0000 1/6-RO/6n RO 0.0000 1/6-RO/6
7- 0,0000 0,0000 1/6-RO/6 0,0000 1/6-RO/6 0,0000 RO 1/6-RO/6
8- 0,0000 0,0000 0,0000 1/6-RO/6 0,0000 1/6-RO/6 1/6-RO/6 RO

If we arbitrarily choose the main diagonal constant input as RO = 0.6, not necessarily zero, then the matrix B reduces to:
B=
1- 0,6000 6,6666E-02 6,6666E-02 0,0000 6,6666E-02 0,0000 0,0000 0,0000
2- 6.6666E-02 0.6000 0.0000 6.6666E-02 0.0000 6.6666E-02 0.0000 0.0000
3- 6.6666E-02 0.0000 0.6000 6.6666E-02 0.0000 0.0000 6.6666E-02 0.0000
4- 0.0000 6.6666E-02 6.6666E-02 0.6000 0.0000 0.0000 0.0000 6.6666E-02

5-6.6666E-02 0.0000 0.0000 0.0000 0.6000 6.6666E-02 6.6666E-02 0.0000
6- 0.0000 6.6666E-02 0.0000 0.0000 6.6666E-02 0.6000 0.0000 6.6666E-02
7- 0,0000 0,0000 6,6666E-02 0,0000 6,6666E-02 0,0000 0,6000 6,6666E-02
8- 0,0000 0,0000 0,0000 6,6666E-02 0,0000 6,6666E-02 6,6666E-02 0,6000

The same treatment followed in the 2D application above applies for the 3D case,

For N sufficiently large The matrix B ^ N converges to zero for any value of RO element of [0,1 [and converges to one for RO = 1

It follows that, only if the BCs are all zeros, then the steady-state equilibrium solution for any initial state is assumed to be the zero vector.

In order for matrix B above to be transformed into an M-Matrix, all of its rows must be changed to sum 1.

On the other hand, an 8x8 Markov matrix with all its row summations equal to unity, one or more of its row summations must be modified to make a sum less than 1.

IV. EIGENVALUES and EIGENVECTORS

We first mention that this article belongs partly to physics and partly to mathematics or more precisely to mathematical physics which means that mathematical matrices and their eigenvalues and eigenvectors have an inherent physical component.

Note that it is necessary here to distinguish 3 notations of different matrices, namely:

i-the basic transition matrix B defined by the conditions i-iv with its eigenvalues evB and ii the transfer matrix E defined by the matrix power summation of equation 4 and iii the transfer matrix D defined by the equality,

D = E-I
with its own evD values.

For the 3 matrices above, we substitute different values of RO from 0 to 1 and calculate the corresponding eigenvalue which is simple since its eigenvector is composed of the constant element vector, (k, k, ..., k) , k other than zero, in other words, for each RO, there is an eigenvalue and an infinite number of eigenvectors. Any vector whose inputs are all equal is an eigenvector.

The table displays the results for evB vs RO.
Table I:
RO: 0 0.1 0.2 0.3 0.4 0.5 0.6. . . . . 0.9 1.0
evB: 0.5 0.55 0.6 0.65 0. 7 0.75 0.8. …. 0.95 1.0

Table I suggests the relationship,
evB = (1+RO)/2 . . . . (6)

Similarly we construct table II for evD vs RO,
Table II
RO = 0 0.1 0.2. . . . . 0.9 1.0
evD = 1 1.22 1.5. . . . . 19 Infinite

Table II suggests the relationship,
evD=(1+RO)/(1-RO) . . . . (7)
Since D = B + B ^ 2 + B ^ 3 +. . . . . .B ^ N.. . . . . (8)
then,
evD = evB + evB ^ 2 +. . . . . .evB ^ N.. . . . . . (9)
In other words, for N sufficiently large ,
(1 + RO) / (1-RO) = (1 + RO) / 2 + [(1 + RO) / 2]^2.. . . . ..+ [(1 + RO) / 2]^N . . . . (10)
that is to say,
Sigma [(1+x)/2]^N from N=1 to infinity is equal to (1+x)/(1-x) for all values of x in the interval [0,1] . . . . . (11)

In the meantime, we have numerically validated an important principle,

[*For positive symmetric physical power matrices, the sum of their eigenvalues is equal to the eigenvalue of their sum of power series*]

The above axiom is useful for computing some statistically important algebraic power series such [(1+x)/2]^N and [(1+2x)/3]^N [7,8]

V. CONCLUSION

The Markov matrix M is based on two conditions and its chains deal exclusively with the future evolution of the initial state of a given system defined by the inputs of the matrix itself. Some improvements of M such as zero main diagonal and symmetry have been shown to be somewhat successful, but they are still not able to handle boundary conditions or source / sink terms, whereas the proposed B transition chains have proposed a statistical physical matrix, can do that.

Therefore, we present in this paper further improvement of the Markov matrix by i-introducing the constant input diagonal RO element of [0,1] and leaving a place for the boundary conditions.

Moreover, the numerical computations of the eigenvalues of the matrices B and D validated the proposed principle:

[For positive symmetric physical power matrices, the sum of their eigenvalues is equal to the eigenvalue of their sum of power series].This results provides an unconventional way of finding summation solutions of many infinite algebraic series such as [(1 + x) / 2] ^ N and [(1+2x)/3)]^N. [7,8]

Finally, we recommend the proposed improvements which are promising in many areas.

N.B. All the calculations in this article must have been carried out using the Author double precision algorithm to ensure maximum precision, as followed by Ref. 9 for example.

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