A Monte Carlo algorithm for efficient large matrix inversion

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Abstract

This paper introduces a new Monte Carlo algorithm to invert large matrices. It is based on simultaneous coupled draws from two random vectors whose covariance is the required inverse. It can be considered a generalization of a previously reported algorithm for hermitian matrices inversion based in only one draw. The use of two draws allows the inversion on non-hermitian matrices. Both the conditions for convergence and the rate of convergence are similar to the Gauss-Seidel algorithm. Results on two examples are presented, a real non-symmetric matrix related to quantitative genetics and a complex non-hermitian matrix relevant for physicists. Compared with other Monte Carlo algorithms it reveals a large reduction of the processing time showing eight times faster processing in the examples studied.

Keywords: Monte Carlo, inverse matrix, Gibbs sampler, sparse matrices.

1 Introduction

The computation of the inverse of a matrix or some of its elements is one of the main topics in numerical analysis. Large sparse matrices can be usually inverted from its factors obtained by using sparse matrix techniques [11]. Although it can be alleviated by reordering rows and columns, these techniques suffer from the fill-in required by the LU factorization and they usually result in algorithms demanding large random access memory (RAM) values.

Monte Carlo algorithms are used to estimate empirically the expectation of random variables. Using them to invert matrices consist basically in obtaining and averaging several realized values of a variable whose expectation is the required inverse. Although Monte Carlo algorithms present a stochastic error, they can be used to obtain estimates of the inverse when the matrix is too large or complicate to be inverted by using conventional or sparse algorithms. These algorithms have high parallel efficiency, they do not demand a great amount of RAM and the processing time is proportional to the number of nonzero elements of the matrix to be inverted. In general, they can be very efficient when rough estimates of the inverse matrix are required.

The most common Monte Carlo algorithms to invert matrices are based on finite discrete Markov chains [2]. In these algorithms several random trajectories are calculated to solve a linear system of equations for each matrix column. Alternatively, there are Monte Carlo methods based on random variables whose expectation is the whole inverse instead one of its columns. Typically the rational is to consider the sought for inverse matrix \( C^{-1} \) as the covariance matrix of a normally distributed random vector,

\[
z \sim N \left(0, C^{-1}\right).
\]

After generating by any Monte Carlo algorithm sampled values of \( z \) (something for which \( C^{-1} \) is not needed but just \( C \)), the inverse matrix is obtained by an estimation of the variances and covariances of the sample.

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Recently the Gibbs sampler [9, 10] algorithm has been proposed to draw \( z \) values from \( \mathbf{C} \) [8, 14]. The procedure consists in updating successively the elements of \( z \) for several cycles by using the formula

\[
  z_i^{(k)} = \phi_i^{(k)} \frac{1}{\sqrt{c_{ii}}} - \frac{1}{c_{ii}} \sum_{j=1}^{i-1} z_j^{(k)} c_{ij} - \frac{1}{c_{ii}} \sum_{j=i+1}^{n} z_j^{(k-1)} c_{ij}
\]

where the subscript \( i \) means the \( i^{th} \) element of \( z \), the superscript \( (k) \) means the \( k^{th} \) cycle and \( \phi \) is an independent random noise drawn from a standard normal distribution. After a given period of convergence usually called the burn-in period, \( z^{(k)} \) will satisfy at each cycle \( E \left( \mathbf{z}^{(k)} \mathbf{z}^\dagger(k) \right) = \mathbf{C}^{-1} \) or \( E \left( \mathbf{z}^{(k)} Q \mathbf{z}^\dagger(k) \right) = tr Q \mathbf{C}^{-1} \) (the \( \dagger \) denotes hermitian conjugate, i.e., transposition and complex conjugation). These expectations will provide the elements of the inverse or linear functions of them respectively. Hereafter, we will denote this algorithm by \( GS \). Although \( GS \) does not provide an independent but a serially correlated set of samples, the convergence is fast and, contrary to Metropolis-like algorithms, it profits of all the draws.

The obvious disadvantage of the algorithms based in Eq. [14] is a rather narrow range of applicability because of the necessary condition of \( \mathbf{C} \) being positive definite. For many statistical applications this is not a problem [12] but it is a serious drawback in Physics applications (for instance in Lattice QCD [17]). The problem can be bypassed by inverting \( \mathbf{C}^\dagger \mathbf{C} \) and applying the result to \( \mathbf{C} \) but this procedure seriously reduces the efficiency. Rather surprisingly this is not the case for the \( GS \) algorithm. Once recourse is made to the Gibbs sampler to implement the covariance matrix rational, the convergence of the algorithm, at least if it is explicitly written as in Eq. [2], is governed by the sampling method and not by the implications of [14]. As we will see, the convergence conditions are then more flexible but still \( \mathbf{C} \) must be symmetric (or hermitian if defined over the complex numbers).

A different approach usually known as stochastic estimation (\( SE \) from now on), avoid this problem [13] by recourse to the repeated solution of linear systems like in the discrete Markov Chain methods mentioned above but this time the number of systems to be solved does not depend on the rank of the matrix to be inverted. The rational is to solve a series of linear systems \( \mathbf{C} \mathbf{v} = \phi \) where \( \phi \) is drawn from a random variable satisfying \( E(\phi) = 0 \) and \( E(\phi \phi^\dagger) = \mathbf{I} \). The inverse is then given by taking the ensemble average \( E(\mathbf{v} \phi^\dagger) = \mathbf{C}^{-1} \). Rather surprisingly it was not recognized until recently that this method do not rely on the gaussianity of \( \phi \). Thus, Dong and Liu [6] and, independently, García-Cortés [7] have shown that the efficiency of the method improves substantially when is drawn as \( \phi_i = 2B - 1 \), where \( B \) is a Bernoulli random variable (a \( Z^2 \) noise).

When applicable, however, it is expected that \( GS \) will be more efficient than \( SE \). This comes from the fact that \( GS \) mimics Gauss-Seidel algorithm but including noise at each cycle [18]. The processing time to obtain each realized value of \( \mathbf{z} \mathbf{z}^\dagger \) or \( \mathbf{z}^\dagger Q \mathbf{z} \) is then slightly greater than the processing time of a Gauss-Seidel iteration, while the processing time to obtain a \( SE \) realized value is equivalent to the processing time needed to solve a linear system.

In this paper we introduce a new "noisy" Gauss-Seidel method which include as a particular case the \( GS \) algorithm. Our algorithm, that we will call it the correlated chains sampling algorithm (\( CC \) from now on), is applicable to nondefinite positive matrices and profits of the larger efficiency of the \( Z^2 \) noise. The power of the algorithm is assessed with two different non-hermitian matrix, a real one used in genetic improvement in animal breeding and a complex one typical of particle Physics. Numerical tests show how our proposal can be around an order of magnitude faster than \( SE \). The sufficient and necessary conditions for the convergence of the method are also given.

2 The correlated chains sampling algorithm

The \( CC \) algorithm introduced in this section is based on the simultaneous update of a couple of random vectors \( \mathbf{z} \) and \( \mathbf{w} \) such as, after convergence of the algorithm, \( E \left( \mathbf{z} \mathbf{z}^\dagger \right) = \mathbf{C}^{-1} \) being \( \mathbf{C} \) the
matrix to be inverted. The algorithm updates simultaneously each element of \( z \) and \( w \) using

\[
z_i^{(k)} = \phi_i^{(k)} \frac{1}{\sqrt{c_{ii}}} - \frac{1}{c_{ii}} \sum_{j=1}^{i-1} z_j^{(k)} c_{ij} - \frac{1}{c_{ii}} \sum_{j=i+1}^{n} z_j^{(k-1)} c_{ij}
\]

(3)

\[
w_i^{(k)} = \phi_i^{(k)} \frac{1}{\sqrt{c_{ii}}} - \frac{1}{c_{ii}} \sum_{j=1}^{i-1} w_j^{(k)} c_{ji} - \frac{1}{c_{ii}} \sum_{j=i+1}^{n} w_j^{(k-1)} c_{ji}
\]

(4)

where \( \Phi^{(k)} \) is a set of independent noise vectors such as

\[
E \left( \Phi^{(k)} \right) = 0
\]

(5)

and

\[
E \left( \Phi^{(k)} \Phi^{(l)\dagger} \right) = I \delta_{k,l}.
\]

(6)

Note that the noise term in (3) and in (4) are both the same.

After discarding \( N \) cycles of a total of \( M \) as a period of convergence or burn-in, the Monte Carlo estimation of the inverse can be obtained from,

\[
C^{-1} \simeq \frac{1}{M - N} \sum_{k=N+1}^{M} z^{(k)} w^{(k)\dagger}.
\]

(7)

Expression \( E(\z^\dagger Q \z) = \text{tr} Q C^{-1} \) also holds, and its Monte Carlo estimation via the CC algorithm is given by

\[
\text{tr} Q C^{-1} \simeq \frac{1}{M - N} \sum_{k=N+1}^{M} \z^{(k)\dagger} Q w^{(k)}
\]

(8)

### 2.1 Demonstration

Let us start by rewriting Eqs. (5) and (6) in matrix form,

\[
z^{(k)} = \frac{1}{\sqrt{D}} \Phi^{(k)} - \frac{1}{D} L z^{(k)} - \frac{1}{D} U z^{(k-1)},
\]

(9)

\[
w^{(k)\dagger} = \Phi^{(k)\dagger} \frac{1}{\sqrt{D}} - \frac{1}{D} U^\dagger w^{(k)} - \frac{1}{D} L^\dagger w^{(k-1)},
\]

(10)

where \( L, D \) and \( U \) are the lower triangle, the diagonal and the upper triangle of \( C \) respectively, so that \( L + D + U = C \). Solving for \( z^{(k)} \) and \( w^{(k)\dagger} \) from Eqs. (9) and (10) we have,

\[
z^{(k)} = \frac{1}{(D + L) \sqrt{D}} \Phi^{(k)} - \frac{1}{D + L} U z^{(k-1)},
\]

(11)

\[
w^{(k)\dagger} = \Phi^{(k)\dagger} \frac{1}{(D + U) \sqrt{D}} - w^{(k-1)\dagger} L \frac{1}{D + U}.
\]

(12)

After running the algorithm during \( n \) updating cycles (11) and (12) leads to,

\[
z^{(n)} = \sum_{k=0}^{n} (-T)^k \Theta^{(n-k)},
\]

(13)

\[
w^{(n)\dagger} = \sum_{k=0}^{n} r^{(n-k)\dagger} (-S)^k,
\]

(14)
where for the ease of the notation we have defined,

\[
T = \frac{1}{D+L} U, \\
S = \frac{1}{D+U},
\]

\[
\Theta^{(k)} = \frac{1}{(D+L)} \sqrt{D} \phi^{(k)},
\]

\[
\Gamma^{(k)} = \frac{1}{(D+U)^{\frac{1}{2}}} \sqrt{D} \phi^{(k)},
\]

for all \( k \) except for \( k = 0 \) for which, again for the ease of notation, \( \Theta^{(0)} \) and \( \Gamma^{(0)} \) denote just the initial vectors \( z^{(0)} \) and \( w^{(0)} \) respectively. For a bounded noise such as the \( Z^2 \) noise, \( z^{(n)} \) and \( w^{(n)} \) are bounded by

\[
\|z^{(n)}\| \leq \left\| \sum_{k=0}^{n} (-T)^k \right\| \left\| \frac{1}{(D+L)} \sqrt{D} \right\| B \leq \left\| \frac{1}{(D+L)} \sqrt{D} \right\| B \sum_{k=0}^{n} \|T^k\|,
\]

\[
\|w^{(n)}\| \leq \left\| \sum_{k=0}^{n} (-S)^k \right\| \left\| \frac{1}{(D+U)} \sqrt{D} \right\| B \leq \left\| \frac{1}{(D+U)} \sqrt{D} \right\| B \sum_{k=0}^{n} \|S^k\|,
\]

where \( B \) is the upper bound of the noise \( \Phi \) and therefore the absolute convergence of the alternating power series \( T \) and \( S \) warrants the convergence of the algorithm. In fact, this is a necessary and sufficient condition for the convergence of the algorithm for any possible value of the noise chain. To see this notice that the worst case corresponds to a noise such as the components of \( T^k \) and \( S^k \) with the maximum absolute values attains positive signs. But the maximum of the absolute values of the components of a matrix is a norm. The convergence of these components, which warrants the convergence of any other of the components, corresponds therefore to the absolute convergence of the series under such a norm and all the norms are equivalent as far as the convergence of matrix series is concerned.

Given the convergence of the alternating power series in \( T \) and \( S \) we have finite \( z^{(\infty)} \) and \( w^{(\infty)} \) and for a given integer \( N \), the \( z^{(n)} \) and \( w^{(n)} \) corresponding to \( n \geq N \) can be split in series of \( N \) terms plus and arbitrarily small remainder for a sufficiently large \( N \),

\[
z^{(n)} = \sum_{k=0}^{N-1} (-T)^k \Theta^{(n-k)} + O(\|T\|^{N+1}),
\]

\[
w^{(n)} = \sum_{k=0}^{N-1} (-S)^k \Gamma^{(n-k)} + O(\|S\|^{N+1}).
\]

The sample average of the \( z w^\dagger \) product discarding \( N \) burn-in cycles of a total of \( M \gg N \), again retaining explicitly only terms up to order \( N \), gives

\[
\langle z w^\dagger \rangle = \frac{1}{M-N} \sum_{n=N}^{M} \sum_{k=0}^{N-1} \sum_{j=0}^{N-1} (-1)^{k+j} T^k \Theta^{(n-k)} \Gamma^{(n-j)} \dagger S^j + O(\|T\|^{N+1}, \|S\|^{N+1}) = \sum_{k=0}^{N-1} \sum_{j=0}^{N-1} (-1)^{k+j} T^k \frac{1}{M-N} \sum_{n=N}^{M} \Theta^{(n-k)} \Gamma^{(n-j)} \dagger S^j + O(\|T\|^{N+1}, \|S\|^{N+1}),
\]

Taking the limit of large \( M \), Eq. (19) yields,
In the limit of large $N$, Eq. (20) reduces to
\[
\lim_{N \to \infty} E(zw^\dagger) = \sum_{k=0}^{N-1} T^k \frac{1}{D + L} \frac{1}{D + U} S^k + O(\|T\|^{N+1}, \|S\|^{N+1}) = \sum_{k=0}^{N-1} T^k \frac{1}{D + L} \frac{1}{D + U} S^k + O(\|T\|^{N+1}, \|S\|^{N+1}).
\]
(20)

Equation (21) represents the stationary value of the $zw^\dagger$ average. That the series in (21) approach $C^{-1}$, when they converge, is easily verified by iteration of the following recursive formula,
\[
\frac{1}{C} = \frac{1}{D + L} D \frac{1}{D + U} + T \frac{1}{C} S,
\]
(22)
which can be derived from the identity,
\[
(C - U) \frac{1}{C} (C - L) = C - (U + L) + U \frac{1}{C} L,
\]
since for the particular case in which $C = D + U + L$ it reduces to,
\[
(D + L) \frac{1}{C} (D + U) = D + U \frac{1}{C} L.
\]

Making use of the definitions (15) and (16) formula (22) follows trivially.

### 2.2 Convergence analysis

As shown in the previous section, the convergence of the algorithm is determined by the absolute convergence of the series,
\[
\sum_{k=0}^{\infty} (-T)^k,
\]
(23)
\[
\sum_{k=0}^{\infty} (-S)^k.
\]
(24)

We therefore center in searching for the necessary and sufficient conditions for the convergence of the series (23) and (24). Restricting the analysis to the series (23) as the same rational applies to (24), first notice that the absolute convergence of (23) implies that the spectral radius of $T$, i.e.,
\[
\lim_{k \to \infty} \|T^k\|^{1/k} \equiv sp(T) \leq 1
\]
is strictly below 1. This comes as a consequence of the Cauchy root convergence test, which implies $\|T^m\|^{1/m} < 1$ for some sufficiently large $m$ if (23) converges. Conversely if $sp(T) < 1$, then $\|T^m\|^{1/m} < 1$ for some large enough $m$ which in turn implies $\|T^m\| < 1$. We now split the series of the absolute values of (23) in a finite part with the terms up to $m - 1$ and the rest, so that,
\[
\sum_{k=0}^{\infty} \|T^k\| = \sum_{k=0}^{m-1} \|T^k\| + \sum_{k=0}^{\infty} \|T^{m+k}\| \leq \sum_{k=0}^{m-1} \|T^k\| + \sum_{k=0}^{\infty} \|T^m\|^k.
\]
Given that $\|T^n\| < 1$ the last term converges to $1/(1-\|T\|)$ and therefore $\|T^n\|$ converges absolutely. Applying the same rationale to (24) we have then, that the algorithm converges in the sense that both $z^{(\infty)}$ and $w^{(\infty)}$ are finite for any possible drawn values of the noise $\Phi$, if and only if $sp(T) < 1$ and $sp(S) < 1$. In strict sense, these are the necessary and sufficient conditions for the convergence of Eqs. (11) and (12). The final algorithm is implemented using (11) and (10) and therefore also the non-singularity of $D$ is needed.

2.3 The burn-in period and Monte Carlo error

As usual in this kind of algorithms, the efficiency of the code is increased by discarding a number of iterations, $N$, called burn-in period, which are too influenced by the initial values. Given that the $CC$ path does not converge to a deterministic value but to a random variable an estimation of $N$ is not as easy as in a deterministic iterative procedures (for instance, the Gauss-Seidel algorithm). To overcome the difficulties associated to the random nature of the algorithm we will use the so-called coupling method [16]. It consists in running a couple of paths for both $z$ and $w^*$ with different initial values but with the same random numbers for each couple. When the difference between paths of a couple reach a given tolerance, the burn-in is assumed to be finished. From (9) the difference between two paths $z_1$ and $z_2$ with different initial values but with the same $\Phi^{(k)}$ results in,

$$z_2^{(k)} - z_1^{(k)} = -\frac{1}{D}L(z_2^{(k)} - z_1^{(k)}) - \frac{1}{D}U(z_2^{(k-1)} - z_2^{(k-1)}) .$$

But Eq. (25) is nothing else that the formula corresponding to a Gauss-Seidel iterative algorithm $\|T^n\|$ for the solution of the linear system,

$$C(z_2 - z_1) = 0,$$

whose solution is $z_2 - z_1 = 0$, for a non-singular $C$. Not surprisingly, the condition for the convergence of the Gauss-Seidel algorithm represented by (25) is, $sp((D + L)^{-1}U) < 1$, that is, $sp(T) < 1$. As expected, the same rationale applied to Eqs. (10) leads to a Gauss-Seidel algorithm for $C^t(w_2 - w_1) = 0$ with a convergence condition $sp((D^t + U^t)^{-1}L^t) < 1$, that is, $sp(S) < 1$. These two Gauss-Seidel procedures can be useful to analyze the convergence rate of the $CC$ algorithm in a given instance.

It is also relevant to calculate the Monte Carlo error of the expectations [7]. The Monte Carlo error is Gaussian because of the central limit theorem, but the realized values provided by the $CC$ algorithm are serially correlated and its Monte Carlo variance is bigger than the Monte Carlo variance expected from an independent set of $M - N$ samples. To calculate the Monte Carlo error instead of $M - N$ samples, we used a higher effective number of samples as proposed in [12].

2.4 Algorithm

Algorithm 1 shows the correlated chains algorithm including the determination of the burn-in period ($N$). During the burn-in period, four chains are computed until the paths converge to a given tolerance, typically a number small enough to avoid the dependency of the chains on the starting values. In order to simplify the algorithm outlined here, we consider a fixed chain length ($M$), i.e., we are assuming that the $M - N$ cycles after burn-in are enough to obtain accurate estimates of the elements of the inverse. Nevertheless, in the numerical tests presented in this paper, we have included the determination of $M - N$ by inserting the calculation of the effective number of cycles during the iteration process.

**Algorithm 1** CORRELATED CHAINS ALGORITHM INCLUDING THE DETERMINATION OF THE BURN-IN PERIOD

*Given n, Q, C, B, tol*

1. Set arbitrary starting values for $z$, $z^*$, $w^*$ and $w'^*$, for instance $z_i=0$, $z_i^*=i$, $w_i=0$ and $w_i^*=i$. 

6
2. Sample $\phi$ as a vector containing independent draws according with definition (5) and (6)
3. Update $z, z^*, w$ and $w^*$ by using equations (3) and (4)
4. $p \leftarrow p + 1$
5. Go to step 2 until $z^T z^* < \text{tol}$ and $w^T w^* < \text{tol}$
6. Sample $\phi$ as a vector containing independent draws according with definition (5) and (6)
7. Update $z$ and $w$ by using equations (3) and (4)
8. Accumulate $z^T Q w$ in $s$
9. Go to step 6 to compute the next round of iteration ($B - p$ times)
10. Set the final estimate: $\text{tr} QC^{-1} \leftarrow s / (B - p)$

3 Numerical tests

To check the computational efficiency of the proposed algorithm we will compare its performance with respect to the efficiency of the SE algorithm which has shown itself as an efficient inversion method [6]. We will make use of two different examples from two disparate fields: genetic improvement in animal breeding and quantum field theory in the lattice.

3.1 Example 1. Wu and Schaeffer’s real asymmetric matrix

The Henderson’s mixed model equations [15] are routinely used in animal breeding to evaluate the candidates to the artificial selection in livestock populations. This method takes into account both the performance records of the animals in a given population and the pedigree relationships between animals. In animal breeding, the quality of the estimations provided by a given model corresponds to the diagonal elements of the inverse of a coefficient matrix. For instance, in the case of the simplest model, these diagonal elements, known as the prediction error variances, take the form

$$\text{diag} \left[ \left( X^\dagger X \begin{bmatrix} X^\dagger & \sigma^2 \end{bmatrix} \begin{bmatrix} X & \mathbf{1} \end{bmatrix} \mathbf{1} \right) \right]^{-1} \sigma^2_e$$

(26)

where $X$ is an incidence matrix mapping animals into herds. Its nonzero elements are $x_{ij} = 1$, which indicates that animal $i$ was recorded in herd $j$. $\mathbf{1}$ is the identity matrix with order equal to the number of animals in the population. Variances $\sigma^2_e$ and $\sigma^2_a$ are assumed to be known and correspond to the additive genetic variance and the residual variance. $\mathbf{A}$ is known as the numerator relationship matrix and it maps the genetic relationships between animals. For instance, $a_{ij} = 0.25$ if animals $i$ and $j$ are half-sibs, $a_{ij} = 0.5$ if animals $i$ and $j$ are parent-progeny related, $a_{ii} = 1$ if the animal $i$ is not inbred, etc. The inverse of the numerator relationship matrix $\mathbf{A}^{-1}$ can be easily obtained by using the Henderson’s rules [15], but the whole coefficient matrix in equation (26) has to be explicitly inverted.

The amount of animals used in a typical analysis is around hundreds of thousands and at least a matrix row per animal is needed so that the rank of the coefficient matrix in Eq. (26) is of that order. This coefficient matrix is positive definite and the Gibbs sampler based algorithm [14] can be easily implemented. Nevertheless, the artificial selection based on the Henderson’s mixed model equations tend to select animals coming from a small number of families and the percentage of inbreeding increases significantly after a few generations of artificial selection. Wu and Schaeffer [19] proposed an original method to select artificially the populations keeping the genetic gain very close to the Henderson’s optimum but reducing significantly the rate of inbreeding. The numerator relationship matrix has to be replaced by a customary asymmetric relationship matrix $\mathbf{\tilde{A}}$, and they provide simple rules to obtain $\mathbf{\tilde{A}}^{-1}$. For each animal $i$ in the pedigree, with sire $s$ and dam $d$,

1. Add $((1 - \lambda) \delta_i + \lambda)$ to the $(i, i)$ position of $\mathbf{\tilde{A}}^{-1}$,
2. Add $-(1 - \lambda) \delta_i/2$ to the $(i, s)$ and $(i, d)$ positions of $\mathbf{\tilde{A}}^{-1}$,
Table 1: Topics of the Wu and Schaeffer’s coefficient matrix in two cases of different size.

| Case | 1     | 2     |
|------|-------|-------|
| Number of animals | 50000 | 100000|
| Number of herds   | 5000  | 10000 |
| Rank of the coefficient matrix | 55000 | 110000|
| Nonzero elements | 424978 | 848982|
| $\sigma_i^2$      | 3.0   | 3.0   |
| $\lambda$         | 0.2   | 0.2   |

3. Add $-\delta_i/2$ to the $(s,i)$ and $(d,i)$ positions of $\tilde{A}^{-1}$.

4. Add $-\delta_i/4$ to the $(s,s)$, $(d,d)$, $(s,d)$ and $(d,s)$ positions of $\tilde{A}^{-1}$,

where $\delta_i = 2$ when both parents of the $i^{th}$ animal are known, $\delta_i = 4/3$ when one parent is known and $\delta_i = 1$ when both parents are unknown. $\lambda \in [0,1]$ is a known coefficient which determine the weight of the family records in each animal genetic evaluation, for instance, setting $\lambda = 0$ correspond to the conventional Henderson’s mixed model equations. These rules result in an asymmetric coefficient matrix for $\lambda \neq 0$, non suitable for GS. Both SE and CC can be used to compute the inverse required in expression (26) even in cases where $A$ is replaced by its non-symmetric counterpart $\tilde{A}$. We will now compare the performance of our algorithm against the $SE$ estimator using two cases of Wu and Schaeffer’s coefficient matrices as described in Table 1.

The correlated chains sampling was implemented by setting the tolerance for burn-in as $5 \times 10^{-5}$. After the burn-in period was finished, realized values of $tr(z^\dagger Qw)$ were obtained for each cycle and averaged. Convergence after burn-in was checked every $100^{th}$ iteration. The standard error of the final estimate of $E[tr(z^\dagger Qw)]$ was obtained from the variance between realized values of $tr(z^\dagger Qw)$ and an effective chain length as described in [12]. Making recourse of this effective length comes as a consequence of the correlated nature of the realized values in the $CC$ algorithm. At any rate, we tested the Geyer’s method against an empirical standard error estimate obtained by replicating one hundred times the whole analysis varying the random seed number. The algorithm was assumed to reach the convergence when the standard error yielded a relative error smaller than the required tolerance of $5 \times 10^{-5}$.

$SE$ method was implemented by solving the linear systems by both the iterative Gauss-Seidel algorithm and the bi-conjugate gradient method. The latter resulted in a more efficient $SE$ algorithm in terms of CPU time and it is the only one presented in this manuscript.

Table 2 shows the results of both algorithms in cases 1 and 2. Relevant topics concerning the computing efficiency of the $CC$ algorithm are the number of rounds computed to reach the burn-in tolerance, the number of rounds required to reach the required standard error of the final estimate, and the CPU time required to compute both each burn-in cycle (four chains) and each after burn-in cycle (two chains). Relevant topics for the $SE$ algorithm are the average number of rounds required to solve each linear system via the bi-conjugate gradient method (maximum change between successive iterations was set to $5 \times 10^{-5}$), the number of linear systems to be solved in order to reach the required standard error of the final estimate and the CPU time per bi-conjugate gradient round of iteration. All CPU times in Table 2 are referred to the time taken to complete a cycle in the $CC$ algorithm in the smallest case.

Table 2 shows also the agreement between the results provided by both the $CC$ and the $SE$ algorithms. The $CC$ algorithm is vastly more efficient in terms of the final CPU time required for the computation of the inverse being around eight times faster then its $SE$ counterpart.

3.2 Example 2. The Dirac’s free fermion complex non-hermitian matrix

We now proceed further in assessing the performance of the $CC$ algorithm by including complex matrix components as well as by strengthen the number of non-zero elements (in the millions range). The tolerance now set to $10^{-5}$ with respect to the absolute value rather than for real and
Table 2: Results of CC and SE on the two Wu and Schaeffer’s matrices

|                  | CC method | SE method |
|------------------|-----------|-----------|
|                  | Case 1    | Case 2    | Case 1    | Case 2    |
| N                | 103       | 104       | Rounds per system | 34.63 | 38.04 |
| M − N            | 39200     | 23800     | Total rounds   | 285732 | 202448 |
| Eff. length size | 15788     | 8163      | Number of systems | 8251 | 5322 |
| $E[tr(z'Qw)]$    | 10371     | 20738     | $E[tr(z'Qw)]$  | 10371 | 20738 |
| $Var[tr(z'Qw)]$  | 3932      | 8123      | $Var[tr(z'Qw)]$ | 2391 | 5301 |
| MC St. error     | 0.499     | 0.998     | MC St. error   | 0.499 | 0.998 |
| Empirical St. error | 0.502 | 1.047     | CPU time per burn-in cycle | 1.97 | 3.99 |
| CPU time per cycle | 2.48 | 5.92      | CPU time per round | 1.03 | 1.99 |
| CPU time per eff. cycle | 2.48 | 5.92    | CPU time per system | 35.69 | 75.80 |
| Total CPU time   | 39403     | 48799     | Total CPU time | 294303 | 402872 |

imaginary part independently. The chosen example is very well representative of the computational demanding tasks typical of the physical sciences. It belongs to the realm of elementary particle physics known as Lattice Quantum Chromodynamics briefly described in the following.

In elementary particle physics the evolution of the particles is described in terms of a field, $\psi(x)$, over the space-time ($x$ is a four components vector, one representing time, the other three the spatial coordinates) which governs the annihilation and creation of particles. More specifically $\psi(x)$ is an operator whose action on the elements of its domain (a Hilbert space) represents the annihilation of a particle at time $x_0$ and spatial coordinates ($x_1, x_2, x_3$). Conversely, the action of the adjoin field $\psi(\dagger)$ (the hermitian conjugate in a matrix representation of $\psi(x)$), describes the creation of a particle at space-time coordinates $x$. For a class of particles called 1/2-spin Fermions, such as the electron, $\psi$ is in turn a four components object (each component being an operator) called a spinor, an object without a classical analog (it is not a vector since under a $2\pi$ rotation changes its sing). Free evolution of such particles, i.e., without interaction with other particles, is governed by the Dirac’s equation which in the so called Euclidean representation reads

$$L \psi \equiv (\partial_\mu \gamma^\mu + m)\psi = 0,$$

(27)

where $m$ is the mass of the particle, $\mu$ runs over the four spatio-temporal coordinates, $\partial_\mu$ denotes derivative along the $\mu$ coordinate, summation over repeated indexes is assumed and $\gamma^\mu$ is a set of four non-hermitian matrices of dimension four satisfying

$$\gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu = 2\delta^{(4)}_{\mu \nu},$$

where $\delta^{(4)}_{\mu \nu}$ denotes a four by four unit matrix multiplied by the standard Kronecker delta. Alternatively the evolution can be described through the associated Green function of Eq. (27), that is, the solution of

$$LG(x,x') = \delta(x-x'),$$

(28)

where $\delta(x-x')$ represents the Dirac’s delta. $G(x,x')$ is known also as a propagator of the field since given an initial configuration for the field $\psi(x^0)$, the field at any other space-time event is obtained by

$$\psi(x) = \int G(x,x^0)\psi(x^0)dx^0,$$

that is, $G(x,x^0)$ represents the propagation of a Dirac’s delta signal from the event $x^0$ to the event $x$. In probabilistic terms, it gives the probability of finding a particle at the space-time event $x$ given that it was at the event $x^0$. Propagators are of paramount importance in quantum field theory.
In general the evolution is far more complicated than that described by (27) since interactions among several fields will be effective. Thus, electrons, having electric charge will interact between each other through the electromagnetic field (a gauge field in the jargon of quantum field theory) or, in terms of particles, by exchange of photons. Eq. (27) must then be supplemented with both a free term for the evolution of photons and an interaction term between photons and electrons. Within this frame (Quantum Electrodynamics) the interaction is weak enough for a perturbative approach in many interesting situations. However, there are other cases in which the coupling is so strong that perturbative techniques are useless. The paradigmatic case is the interaction of quarks (also fermions, like the electrons) inside nucleons (protons and neutrons), this time by exchange of particles called gluons describing an interaction known as Quantum Chromodynamics (QCD). In such a case, recourse is made to a discretization of the space-time (a space-time lattice) suitable for a numerical solution of the problem. Under such discretization Eq. (28) leads to a matrix equation of the form \( L G = I \), so that the propagator is given by \( L^{-1} \). Interactions make \( L \) depend on the value of the gluon field at each spacetime event but still the discretized quark propagator is given by a matrix inversion. However, an extra average over an ensemble of different realizations of the fields is necessary. Altogether leads to an extremely demanding computational task and Lattice QCD is responsible of a major part of the CPU time consumed in Science (for a series of reviews in the computational aspects of Lattice QCD see [3] and in particular [13]). Here we are only interested in testing the CC algorithm so that we restrict ourselves to the free case described by (27). Although trivial from the physical point of view, this simple case can be solved analytically [4] and therefore the solution can be checked. The final result after certain technical details reads (in a compact notation) [4],

\[
L_{mn} = \delta^{(4)}_{mn} + K \sum_{\mu} \left( (1 + \gamma^\mu) \delta^{(4)}_{m+\delta_{\mu},n+\delta_{\mu}} + (1 - \gamma^\mu) \delta^{(4)}_{m-\delta_{\mu},n+\delta_{\mu}} \right),
\]  

(29)

where Latin indexes run over lattice points, Greek indexes over space-time dimensions, \( K \) is a constant approaching 1/8 in the continuum limit and \( \delta_{\mu\nu} \) is the standard Kronecker delta. In this notation a Latin index, say \( m \), labels a lattice point while the \( \nu \) spatio-temporal coordinate of such a point is denoted by \( m_\nu \). Thus, in each lattice point a four dimensional matrix acting on the spinor components is defined.

Explicitly in terms of both the spatio-temporal coordinates (Latin indexes) and spinor components (Greek indexes) \( L \) reads

\[
L_{\mu\nu a b c d m n l k} = \delta_{\mu\nu} \delta_{a m} \delta_{b n} \delta_{c l} \delta_{d k} + K \left\{ \delta_{b n} \delta_{c l} \delta_{d k} \left[ \delta_{a+1 m} \left( \delta_{\mu\nu} + \gamma^1_{\mu\nu} \right) + \delta_{a-1 m} \left( \delta_{\mu\nu} - \gamma^1_{\mu\nu} \right) \right] + \cdots \right\}. 
\]  

(30)

In the next term in the sum \( \gamma^1 \) changes to \( \gamma^2 \), \( a \) interchanges with band \( m \) with \( n \) and so for until the indexes are exhausted. The \( \gamma \)'s matrices are defined as

\[
\gamma^i = \begin{pmatrix} 0 & \sigma^i \\ \sigma^i & 0 \end{pmatrix}, \quad i = 1, 2, 3
\]

and

\[
\gamma^4 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}
\]

where the \( \sigma \)'s, the 1 and the 0 must be understood as two by two matrices. The \( \sigma \)'s are the show called Pauli matrices given by

\[
\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},
\]

\[
\sigma^2 = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix},
\]
\[ \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \]

with \( i \) representing the imaginary unit. Eq. (30) is useful to implement \( L \) in a program but to apply the \( CC \) algorithm as described in section 2.4, a one to one mapping of the ten indexes of \( L \) to only two is also needed. We use the following one usual in QCD

\[
m' = 1 + a + N_1 (b + N_2 (c + N_3 (d + N_0 \mu))) \]
\[
n' = 1 + m + N_1 (n + N_2 (l + N_3 (k + N_0 \nu))),
\]

Here \( N_1, N_2, N_3 \) and \( N_0 \) are the number of discrete points in each spatio-temporal coordinate of the lattice (as above, 0 corresponds to the time coordinate). The rank of the corresponding matrix is then \( 4 N_0 N_1 N_2 N_3 \) while expression (30) yields fourteen non zero elements per row so that the total number of non zero elements is \( 56 N_0 N_1 N_2 N_3 \).

Again two cases were tested. The parameters are given in table 3 and corresponds to two different spatio-temporal lattice sizes in both cases with the same number of discrete values for the four coordinates. The value of \( K \) was arbitrarily chosen to 0.1.

| Case | 1 | 2 |
|------|---|---|
| \( N_1, N_2, N_3, N_0 \) | 18 | 20 |
| Rank of \( C \) | 419904 | 640000 |
| Nonzero elements | 5878656 | 8960000 |

Table 4: Results of \( CC \) and \( SE \) on Dirac’s matrices (first case).

| \( CC \) method | \( SE \) method |
|-----------------|----------------|
| \( N \) | 18 | Rounds per system | 55.03 |
| \( M - N \) | 10832 | Total rounds | 219167 |
| Eff. length size | 10805.0 | Number of systems | 3983 |
| \( E \left[ tr(z^\dagger Qw) \right] \) exact value | 413007.84+0i | 413005.08-1.98i |
| \( E \left[ tr(z^\dagger Qw) \right] \) | 413004.47-1.87i | 413005.08-1.98i |
| \( Var \left[ tr(z^\dagger Qw) \right] \) | 184130.43 | 67827.29 |
| MC St. error | 4.128 | MC St. error | 4.130 |
| CPU time per burn-in cycle | 1.43 | |
| CPU time per cycle | 0.4746 | CPU time per round | 0.40 |
| CPU time per eff. cycle | 1.00 | CPU time per system | 21.89 |
| Total CPU time | 10859 | Total CPU time | 87167 |
Table 5: Results of CC and SE on Dirac’s matrices (second case).

|                      | CC method                | SE method                 |
|----------------------|--------------------------|---------------------------|
| N                    | 18                       | 56.08                     |
| M − N                | 6782                     | 146379                    |
| Eff. length size     | 6848.8                   | 2610                      |
| E \( | tr(z^i Qw) | \) exact value           | 629489.14+0i              |
| E \( | tr(z^i Qw) | \)                        | 629482.78-0.11            |
| Var \( | tr(z^i Qw) | \)                      | 270373.73                 |
| Var \( | tr(z^i Qw) | \)                      | 103395.82                 |
| MC St. error         | 6.283                    | 6.294                     |
| CPU time per burn-in cycle | 2.26                  |                           |
| CPU time per cycle   | 1.54                     | 0.61                      |
| CPU time per eff. cycle | 1.53                   | 33.99                     |
| Total CPU time       | 10503                    | 88721                     |

From inspection of tables 4 and 5 it is clear the advantage of the CC algorithm whose performance again is around eight times higher than that of the SE. As explained above, this time it is possible to check the results against exact deterministic calculations. As expected they coincide with the estimated values within the imposed tolerance.

4 Discussion and Conclusion

Once the far superior efficiency of the CC algorithm has been demonstrated some comments about its applicability seems in order but first a note about the GS. Notice that the GS as implemented in [2] is just the particular case of CC corresponding to hermitian matrices since in this case \( z^i = w \). Therefore its convergence is determined by \( sp(T) < 1 \) and the no singularity of \( D \). These conditions do not implies \( C \) being positive definite. For instance, in the trivial case of \( C \) being diagonal, \( sp(T) = 0 \), and Eq. [2] reduces to \( z_{i1}^{(k)} = \phi_{i1}^{(k)} / \sqrt{c_{11}} \) which, although implies imaginary values of \( z_{i1}^{(k)} \) works perfectly.

In the general case when the convergence criteria are not satisfied at least two alternatives exits. One is to rewrite the algorithm with a different partition than that shown here. For instance, suppose that \( D \) is singular. Then, a possibility is to use a partition with relatively small non singular diagonal blocks surrounding the zeros of \( D \), amenable of been inverted deterministically with the memory recourses available. In fact, in terms of time efficiency, there will be partitions more efficient than the one used here but, obviously, without the appealing implementation simplicity of Eqs. [3] and [4]. As a rule of the thumb, the convergence will be guaranteed for a sufficiently “heavy” \( D \). A new partition in the way just described could solve problems with small elements in the original \( D \) not only with zeros.

Another simpler possibility is just to reorder the rows and the columns of \( C \) trying to locate in the diagonal large enough elements. In general, reordering which implies a low time penalty, could be advantageous to improve the convergence of the method.

In summary, we have presented an efficient stochastic algorithm based in correlated Markov chains suitable for the inversion of very large matrix whenever the memory recourses are not enough for the application of the standard deterministic methods. The efficiency of the algorithm has been tested in a couple of numerical examples rendering a dramatic improving of eight times faster runs with respect to the best stochastic method known by the authors. The necessary and sufficient conditions for the convergence of the algorithm have been also given.

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