Determinant Approximations

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SUMMARY

A sequence of approximations for the determinant and its logarithm of a complex matrix is derived, along with relative error bounds. The determinant approximations are derived from expansions of $\det(X) = \exp(\operatorname{trace}(\log(X)))$, and they apply to non-Hermitian matrices. Examples illustrate that these determinant approximations are efficient for lattice simulations of finite temperature nuclear matter, and that they use significantly less space than Gaussian elimination.

The first approximation in the sequence is a block diagonal approximation; it represents an extension of Fischer's and Hadamard's inequalities to non-Hermitian matrices. In the special case of Hermitian positive-definite matrices, block diagonal approximations can be competitive with sparse inverse approximations. At last, a different representation of sparse inverse approximations is given and it is shown that their accuracy increases as more matrix elements are included. Copyright © 2005 John Wiley & Sons, Ltd.

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1. Introduction

For a complex matrix we present approximations for the determinant and its logarithm, together with error bounds.

The approximations were motivated by a problem in computational quantum field theory: the simulation of finite temperature nuclear matter on a lattice [16]. In this application, the logarithm of the determinant is desired to 2-3 significant digits. The matrices are sparse, and non-Hermitian. Because the desired accuracy is low, LU decomposition with partial pivoting [12, §14.6], [21, §3.18] is too costly. Since the matrices are not Hermitian positive-definite, sparse approximate inverses [19], Gaussian quadrature based methods [3], and Monte Carlo methods [19, §4] or hybrid Monte Carlo methods [7, 10, 20] do not apply. Monte Carlo and

quadrature-based methods can be extended to non-Hermitian matrices, however then the sign of the determinant is usually lost, e.g. [2, §3.2.3].

To approximate the determinant $\det(M)$ we decompose $M = M_D + M_{\text{off}}$ such that M_D is a non-singular matrix. Then $\det(M) = \det(M_D) \det(I + M_D^{-1} M_{\text{off}})$, where I is the identity matrix. In

$$\det(I + M_D^{-1} M_{\text{off}}) = \exp(\operatorname{trace}(\log(I + M_D^{-1} M_{\text{off})))),$$

we expand $\log(I + M_D^{-1} M_{\text{off}})$, obtaining a sequence of increasingly accurate approximations. Error bounds for these approximations depend on the spectral radius of $M_D^{-1} M_{\text{off}}$.

Overview

The determinant approximations and their error bounds are presented in §2. Approximations from block diagonals (§2.1) are extended to a sequence of higher order approximations (§2.2). They simplify for checkerboard matrices (§2.3) which occur in the neutron matter simulations in [16]. Comparisons with sparse inverse approximations of determinants, which are limited to Hermitian positive-definite matrices (§3) illustrate the competitiveness of block diagonal approximations. As expected, the accuracy of sparse inverse approximations increases as more matrix elements are included. Numerical results with matrices from nuclear matter simulations (§4) show that determinant approximations of desired accuracy can be obtained fast, in 1-3 iterations; and that they require significantly less space than Gaussian elimination (with partial or complete pivoting).

Notation

The eigenvalues of a complex square matrix A are $\lambda_j(A)$, and the spectral radius is $\rho(A) \equiv \max_j |\lambda_j(A)|$. The identity matrix is I, and A^* is the conjugate transpose of A. We denote by $\log(X)$ and $\exp(X)$ the logarithm and exponential function of a matrix X, and by $\ln(x)$ and e^x the natural logarithm and exponential function of a scalar x.

2. Determinant Approximations

We present approximations to the determinant and its logarithm, as well as error bounds.

2.1. Diagonal Approximations

We present relative error bounds for the approximation of the determinant by the determinant of a block diagonal. Let M be a complex square matrix of order n partitioned as a $k \times k$ block matrix

$$M = \begin{pmatrix} M_{11} & M_{12} & \dots & M_{1k} \\ M_{21} & M_{22} & \dots & M_{2k} \\ \vdots & \ddots & \ddots & \vdots \\ M_{k1} & M_{k2} & \dots & M_{kk} \end{pmatrix},$$

where the diagonal blocks M_{jj} are square but not necessarily of the same dimension. Analogously, decompose $M = M_D + M_{\text{off}}$ into diagonal blocks M_D and off-diagonal blocks

M_{off},

$$M_D = \begin{pmatrix} M_{11} & & & \\ & M_{22} & & \\ & & \ddots & \\ & & & M_{kk} \end{pmatrix}, \qquad M_{\text{off}} = \begin{pmatrix} 0 & M_{12} & \ldots & M_{1k} \\ M_{21} & 0 & \ldots & M_{2k} \\ \vdots & \ddots & \ddots & \vdots \\ M_{k1} & M_{k2} & \ldots & 0 \end{pmatrix}. \qquad (1)$$

The block diagonal matrix M_D is called a pinching of M [4, §II.5]. We consider the approximation of $\det(M)$ by the determinant of a pinching, $\det(M_D)$; and in particular bounds of the form $\det(M) \leq \det(M_D)$. The matrices for which such bounds are known to hold are characterized by eigenvalue monotonicity of the following kind.

A complex square matrix M is a τ-matrix if [8, pp 156-57]:

1. Each principal submatrix of M has at least one real eigenvalue.
2. If S_1 is a principal submatrix of M and S_{11} a principal submatrix of S_1 then $\lambda_{\min}(S_1) \leq \lambda_{\min}(S_{11})$, where $\lambda_{\min}$ denotes the smallest *real* eigenvalue.
3. $\lambda_{\min}(M) \geq 0$.

The class of τ-matrices includes Hermitian positive-definite, M-matrices and totally non-negative matrices [8, pp 156-57], [18, Theorem 1].

Hadamard-Fischer Inequality. If M is a τ-matrix then [8, Theorem 4.3]

$$\det(M) \leq \det(M_D). \qquad (2)$$

Strictly speaking, (2) is called a Hadamard-Fischer inequality only for $k = 2$ [8, (0.5)]. If $k = 2$ and M is Hermitian positive-definite then (2) is Fischer's inequality [13, Theorem 7.8.3]. If $k = n$ and M Hermitian positive-definite then (2) is Hadamard's inequality [6, Theorem 8], [13, Theorem 7.8.1]. Extensions of (2) to generalized Fan inequalities are derived in [17, 18]. The Hadamard-Fischer inequality (2) implies the obvious relative error bound for the determinant of a pinching,

$$0 < \frac{\det(M_D) - \det(M)}{\det(M_D)} \leq 1.$$

In the theorem below we tighten the upper bound.

Theorem 1. *Let M be a complex matrix of order n. If $\det(M)$ is real, M_D is non-singular with $\det(M_D)$ real, and all eigenvalues $\lambda_j(M_D^{-1} M_{\text{off}})$ are real with $\lambda_j(M_D^{-1} M_{\text{off}}) > -1$, then*

$$0 < \frac{\det(M_D) - \det(M)}{\det(M_D)} \leq 1 - e^{-\frac{n\rho^2}{1+\lambda_{\min}}},$$

where $\rho \equiv \rho(M_D^{-1} M_{\text{off}})$ and $\lambda_{\min} \equiv \min_{1 \leq j \leq n} \lambda_j(M_D^{-1} M_{\text{off}})$.

Proof. Write $\det(M) = \det(M_D) \det(I + A)$, where $A \equiv M_D^{-1} M_{\text{off}}$. Since $I + A$ is non-singular, [14, Theorem 6.4.15(a)] and [14, Problem 6.2.4] imply $\det(I + A) = \exp(\text{trace}(\log(I + A)))$. Furthermore, $\log(I + A) = \sum_{p=1}^{\infty} \frac{(-1)^{p-1}}{p} A^p$ [15, (7) in §9.8]. Hence

$$\det(I + A) = \exp\left(\sum_{j=1}^{n} \ln(1 + \lambda_j(A)) \right).$$

Because $\lambda_j(A) > -1$, $1 \le j \le n$, we can apply the inequality $\frac{\lambda}{1+\lambda} \le \ln(1+\lambda) \le \lambda$ [1, 4.1.33] to obtain

$$\exp(\text{trace}(A))\, e^{-\frac{n\rho(A)^2}{1+\lambda_{\min}}} \le \det(I + A) \le \exp(\text{trace}(A)).$$

At last use the fact that M_D is block diagonal and $\text{trace}(M_{\text{off}}) = \text{trace}(A) = 0$. $\quad\square$

The upper bound for the relative error is small if the eigenvalues of $M_D^{-1}M_{\text{off}}$ are small in magnitude but not too close to -1. The pinching $\det(M_D)$ can be a bad approximation to $\det(M)$ when $I + M_D^{-1}M_{\text{off}}$ is close to singular. If $\det(M_D) > 0$ then Theorem 1 implies a lower bound for $\det(M)$,

$$e^{-\frac{n\rho^2}{1+\lambda_{\min}}} \det(M_D) \le \det(M) \le \det(M_D).$$

In the argument of the exponential function in Theorem 1 we have $\lambda_{\min} < 0$ because $M_D^{-1}M_{\text{off}}$ has a zero diagonal so that $\text{trace}(M_D^{-1}M_{\text{off}}) = 0$. Hence $n\rho^2/(1 + \lambda_{\min}) > n\rho^2$.

Corollary 1. *Theorem 1 holds for Hermitian positive-definite matrices. In particular, Theorem 1 implies error bounds for Fischer's and Hadamard's inequalities.*

The following example shows that $|\det(M)| \le |\det(M_D)|$ may not hold when $M_D^{-1}M_{\text{off}}$ has complex eigenvalues, or real eigenvalues smaller than -1.

Example 1. *Even if all eigenvalues of $M_D^{-1}M_{\text{off}}$ satisfy $|\lambda_j(M_D^{-1}M_{\text{off}})| < 1$, it is still possible that $|\det(M)| > |\det(M_D)|$ if some eigenvalues are complex.*
Consider

$$M = \begin{pmatrix} 1 & \alpha \\ \alpha & 1 \end{pmatrix}, \qquad M_D = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad M_{\text{off}} = \begin{pmatrix} 0 & \alpha \\ \alpha & 0 \end{pmatrix} = M_D^{-1}M_{\text{off}}.$$

Then $\lambda_j(M_D^{-1}M_{\text{off}}) = \pm\alpha$, and $\det(M) = 1 - \alpha^2$. Choose $\alpha = \frac{1}{2}\imath$, where $\imath = \sqrt{-1}$. Then both eigenvalues of $M_D^{-1}M_{\text{off}}$ are complex, and $|\lambda_j(M_D^{-1}M_{\text{off}})| < 1$. But $\det(M) = 1.25 > 1 = \det(M_D)$.
The situation $\det(M_D) > \det(M)$ can also occur when $M_D^{-1}M_{\text{off}}$ has a real eigenvalue that is less than -1. If $\alpha = 3$ in the matrices above then one eigenvalue of $M_D^{-1}M_{\text{off}}$ is -2, and $|\det(M)| = 8 > \det(M_D) = 1$. In general, $|\det(M)|/\det(M_D) \to \infty$ as $|\alpha| \to \infty$.

This example illustrates that, unless the eigenvalues of $M_D^{-1}M_{\text{off}}$ are real and greater than -1, $\det(M_D)$ is, in general, not a bound for $\det(M)$. In the case of complex eigenvalues, however, we can still determine how well $\det(M_D)$ *approximates* $\det(M)$. Below is a relative error bound for the case when M is 'diagonally dominant', in the sense that the eigenvalues of $M_D^{-1}M_{\text{off}}$ are small in magnitude.

Theorem 2 (Complex Eigenvalues). *Let M be a complex matrix of order n. If M_D is non-singular and $\rho \equiv \rho(M_D^{-1}M_{\text{off}}) < 1$ then*

$$\frac{|\det(M) - \det(M_D)|}{|\det(M_D)|} \le c\rho\, e^{c\rho}, \qquad \text{where} \quad c \equiv -n\ln(1-\rho).$$

If also $c\rho < 1$ then

$$\frac{|\det(M) - \det(M_D)|}{|\det(M_D)|} \le \frac{7}{4}c\rho.$$

Proof. This is a special case of Theorem 3.   □

Corollary 2. *Theorem 2 holds for the following classes of matrices: M-matrices; Hermitian positive-definite matrices if $k = n$; Hermitian positive definite block tridiagonal matrices with equally-sized blocks of dimension n/k.*

Proof. In all cases $\rho(M_D^{-1} M_{\text{off}}) < 1$.   □

In the special case of strictly diagonally dominant matrices, Theorem 2 leads to a bound for the approximation of $\det(M)$ by the product of the diagonal elements.

Corollary 3. *If the complex square matrix $M = (m_{ij})_{1 \leq i,j \leq n}$ is strictly row diagonal dominant then*

$$\frac{|\det(M) - \prod_{i=1}^{n} m_{ii}|}{|\prod_{i=1}^{n} m_{ii}|} \leq c\rho \, e^{c\rho}, \qquad \text{where} \quad \rho \leq \max_{i} \sum_{j=1, j \neq i}^{n} \left| \frac{m_{ij}}{m_{ii}} \right|, \quad c \equiv -n \ln(1 - \rho).$$

If also $c\rho < 1$ then

$$\frac{|\det(M) - \prod_{i=1}^{n} m_{ii}|}{|\prod_{i=1}^{n} i m_{ii}|} \leq \frac{7}{4} c\rho.$$

Proof. This is a consequence of Gerschgorin's theorem [9, Theorem 7.2.1].   □

Corollary 3 implies that the product of diagonal elements is a good approximation for $\det(M)$ if M is strongly diagonally dominant.

2.2. A Sequence of General Higher Order Approximations

We extend the diagonal approximations in §2.1 to a sequence of more general approximations that become increasingly more accurate. These approximations, called 'zone determinant approximations' in [16], are justified in the context of nuclear matter simulations. As before, decompose $M = M_D + M_{\text{off}}$ into diagonal blocks M_D and off-diagonal blocks M_{off} (actually, our results hold for any decomposition $M = M_0 + M_E$ where M_0 is non-singular and $\rho(M_0^{-1} M_E) < 1$). Below we give a sequence of approximations δ_m for $\ln(\det(M))$ and Δ_m for $\det(M)$, as well as absolute bounds for δ_m and relative bounds for Δ_m. An absolute bound for the logarithm suffices because $\ln(\det(M)) > 1$ in our applications.

Theorem 3. *Let $M = M_D + M_{\text{off}}$ be a complex matrix of order n, M_D be non-singular and $\rho \equiv \rho(M_D^{-1} M_{\text{off}}) < 1$. Define*

$$\delta_m \equiv \ln(\det(M_D)) + \sum_{p=1}^{m} \frac{(-1)^{p-1}}{p} \text{trace}((M_D^{-1} M_{\text{off}})^p), \qquad \Delta_m \equiv e^{\delta_m}, \qquad m \geq 1.$$

Then

$$|\ln(\det(M)) - \delta_m| \leq c\rho^m, \qquad \frac{|\det(M) - \Delta_m|}{|\Delta_m|} \leq c\rho^m \, e^{c\rho^m}$$

where $c \equiv -n \ln(1 - \rho)$. If also $c\rho^m < 1$ then

$$\frac{|\det(M) - \Delta_m|}{|\Delta_m|} \leq \frac{7}{4} \, c \, \rho^m.$$

Proof. As in the proof of Theorem 1 $\det(M) = \det(M_D)\det(I + A)$, where $A \equiv M_D^{-1}M_{\text{off}}$ and $\log(I + A) = \sum_{p=1}^{\infty} \frac{(-1)^{p-1}}{p}A^p$. Hence

$$\text{trace}\left(\log(I + A)\right) = \sum_{p=1}^{\infty} \frac{(-1)^{p-1}}{p}\text{trace}(A^p).$$

Define the truncated sums

$$L_m \equiv \sum_{p=1}^{m} \frac{(-1)^{p-1}}{p}\text{trace}(A^p), \qquad D_m \equiv e^{L_m}, \qquad m \geq 1.$$

Then

$$\text{trace}\left(\log(I + A)\right) = L_m + z, \qquad z \equiv \sum_{i=1}^{n}\left\{\ln(1 + \lambda_i(A)) - \sum_{p=1}^{m} \frac{(-1)^{p-1}}{p}\lambda_i(A)^p\right\}.$$

Applying to each of the n terms the inequality

$$\left|\ln(1 + \lambda) - \sum_{p=1}^{m} \frac{(-1)^{p-1}}{p}\lambda^p\right| \leq -\ln(1 - |\lambda|)\,|\lambda|^m$$

[1, 4.1.24], [1, 4.1.38] gives $|\ln(\det(I + A)) - L_m| \leq c\rho^m$. The first bound follows now with $\delta_m = \ln(\det(M_D)) + L_m$.

From the first bound, the fact that $\det(I + A) = D_m e^z$, and $|e^z - 1| \leq |z|\,e^{|z|}$ [1, 4.2.39] follows

$$\frac{|\det(I + A) - D_m|}{|D_m|} \leq c\rho^m\,e^{c\rho^m}.$$

We get the second bound from $\Delta_m = \det(M_D)\,D_m$.

If also $c\rho^m < 1$ then [1, 4.2.38]

$$\frac{|\det(I + A) - D_m|}{|D_m|} \leq \frac{7}{4}c\,\rho^m.$$

$\square$

The accuracy of the approximations in Theorem 3 is determined by the spectral radius ρ of $M_D^{-1}M_{\text{off}}$. In particular, the absolute error bound for the approximation δ_m is proportional to ρ^m, hence the approximations tend to improve with increasing m. The numerical results in Sections 3 and 4 illustrate that the pessimistic factor in the bound $|\ln(\det(M)) - \delta_m| \leq -n\ln(1 - \rho)\,\rho^m$ is n. We found that replacing n by the number of eigenvalues whose magnitude is close to ρ makes the bound tight. The approximations for the logarithm can be determined from successive updates

$$\delta_0 \equiv \ln(\det(M_D)), \qquad \delta_m = \delta_{m-1} + \frac{(-1)^{m-1}}{m}\text{trace}((M_D^{-1}M_{\text{off}})^m), \qquad m \geq 1,$$

and $\Delta_m = e^{\delta_m}$. Note that $e^{\delta_0} = \det(M_D)$ is the block diagonal approximation from (1). Hence Theorem 2 is a special case of Theorem 3 with $m = 1$. If a block diagonal determinant approximation is sufficiently accurate, as in §4, it can be much cheaper to compute than a determinant via Gaussian elimination.

2.3. Checkerboard Matrices

For this particular class of matrices, which occurs in our applications [16], every other determinant approximation Δ_m has increased accuracy. We call a matrix M with equally sized blocks M_{ij} of dimension n/k in (1) an *odd checkerboard matrix* (with regard to the block size n/k) if $M_{ij} = 0$ for i and j both even or both odd, $1 \le i, j \le k$; and an *even checkerboard matrix* if $M_{ij} = 0$ for i odd and j even or vice versa. An odd checkerboard matrix has zero diagonal blocks, hence its trace is zero.

Theorem 4. *If, in addition to the conditions of Theorem 3, M_{off} is an odd checkerboard matrix then*

$$\delta_0 = \ln(\det(M_D)), \qquad \delta_m = \begin{cases} \delta_{m-1} & \text{if } m \text{ is odd} \\ \delta_{m-2} - \text{trace}\left(\frac{(M_D^{-1}M_{\text{off}})^m}{m}\right) & \text{if } m \text{ is even.} \end{cases}$$

Proof. If A and B are odd checkerboard matrices (with regard to the same block size) then AB is an even checkerboard matrix. If A is an odd checkerboard matrix and B an even checkerboard matrix then AB and BA are odd checkerboard matrices.

Since $M_D^{-1}M_{\text{off}}$ is an odd checkerboard matrix, so are the powers $(M_D^{-1}M_{\text{off}})^p$ for odd p. This means trace $\left((M_D^{-1}M_{\text{off}})^p\right) = 0$ for odd p. Hence the approximations in Theorem 3 satisfy $\delta_m = \delta_{m-1}$ for m odd. For m even

$$\delta_m = \delta_{m-2} + \left(\frac{(-1)^{m-1}}{m} \text{ trace}\left((M_D^{-1}M_{\text{off}})^m\right)\right) = \delta_{m-2} - \left(\frac{\text{trace}\left((M_D^{-1}M_{\text{off}})^m\right)}{m}\right).$$

$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\square$

Theorem 4 shows that an odd-order approximation is equal to the previous even-order approximation. Hence the even-order approximations gain one order of accuracy.

3. Comparison with Sparse Inverse Approximations

In the special case of Hermitian positive-definite matrices, we illustrate that block-diagonal determinant approximations (see Corollary 1) can compare favourably with approximations based on sparse approximate inverses [19]. We also show that the accuracy of sparse inverse approximations increases when more matrix elements are included.

Idea. To understand how sparse inverse approximations work, we first consider a representation of the determinant based on minors of the inverse [13, §0.8.4]. If M is Hermitian positive-definite of order n, and M_i is the leading principal submatrix of order i of M, then [13, §0.8.4] $\det(M) = \det(M_{n-1})/\sigma_n$, where $\sigma_n \equiv (M^{-1})_{nn}$ is the trailing diagonal element of M^{-1}. Using this expression recursively for $\det(M_{n-1})$ gives

$$\det(M) = \prod_{i=1}^{n} \frac{1}{\sigma_i}, \qquad \text{where} \quad \sigma_i = (M_i^{-1})_{ii}.$$

Determinant approximations based on sparse approximate inverses replace *leading* principal submatrices M_i by just principal submatrices S_i. Specifically [19, §3.2], let M be Hermitian

positive-definite, and let S_i be a principal submatrix of M_i, such that S_i includes at least row i and column i of M. The two extreme cases are $S_i = m_{ii}$ and $S_i = M_i$. In any case, m_{ii} is the trailing diagonal element of S_i, i.e. $S_{n_i,n_i} = m_{ii}$, where n_i is the order of S_i, $1 \leq n_i \leq i$. Let σ_i be the trailing diagonal element of S_i^{-1}, i.e. $\sigma_i = (S_i^{-1})_{n_i,n_i}$. In particular $\sigma_1 = m_{11}^{-1}$. Given n such submatrices S_i, $1 \leq i \leq n$, the sparse inverse approximation of $\det(M)$ is defined as [19, Algorithm 3.3].

$$\sigma \equiv \prod_{i=1}^{n} \frac{1}{\sigma_i}. \tag{3}$$

The sparse approximate inverse method performs Cholesky decompositions $S_i = L_i L_i^*$, where L_i is lower triangular, $2 \leq i \leq n$, and computes $1/\sigma_i = ((L_i)_{n_i,n_i})^2$.

Monotonicity. We show monotonicity of the sparse inverse approximations in the following sense: If the dimensions of the submatrices S_i are increased then the determinant approximations can only become better.

Lemma 1. *If*

$$M = \begin{matrix} & m & k \\ m & \\ k \end{matrix} \begin{pmatrix} A & B \\ B^* & S \end{pmatrix}$$

is Hermitian positive-definite then $(S^{-1})_{ii} \leq (M^{-1})_{m+i,m+i}$, $1 \leq i \leq k$.

Proof. The proof follows from [5, (4)] and the Shermann-Morrison formula [9, (2.1.4)]. $\square$

Lemma 1 implies the following lower and upper bounds for sparse inverse approximations; the lower bound was already derived in [19, (3.25)].

Corollary 4. *If M is Hermitian positive-definite and σ is a sparse inverse approximation in (3) then*

$$\det(M) \leq \sigma \leq \prod_i m_{ii}.$$

Corollary 4 implies that the product of diagonal elements cannot approximate the determinant more accurately than a sparse inverse approximation. Another consequence of Lemma 1 is the monotonicity of the sparse inverse approximation in the following sense: If a principal submatrix $\hat{S}_j$ is replaced by a larger principal submatrix S_j then the determinant approximation can only become better.

Theorem 5. *Let M be Hermitian positive-definite of order n. If for some $1 < j \leq n$, S_j is a principal submatrix of M_j, and in turn $\hat{S}_j$ is a principal submatrix of S_j then*

$$\det(M) \leq \prod_{i=1}^{n} \frac{1}{\sigma_i} \leq \frac{1}{\hat{\sigma}_j} \prod_{i=1, i \neq j}^{n} \frac{1}{\sigma_i}$$

where $\hat{\sigma}_j$ is the trailing diagonal element of $\hat{S}_j^{-1}$.

The next example of block diagonal matrices illustrates that sparse inverse approximations can be inaccurate, even when sparsity is exploited to full extent.

Block-Diagonal Matrices. Let

$$M = \begin{pmatrix} T_3 & & \\ & \ddots & \\ & & T_3 \end{pmatrix}$$

be a block diagonal matrix of order $n = 3k$ with $n/3$ diagonal blocks

$$T_3 \equiv \begin{pmatrix} 3/2 & -1 & \\ -1 & 3/2 & -1 \\ & -1 & 3/2 \end{pmatrix}.$$

The obvious block diagonal approximation (1) with $k = n/3$ gives the exact determinant $\det(M_D) = \det(M) = \det(T_3)^{n/3} = (3/8)^{n/3}$. For the sparse inverse approximation (3) we choose the submatrices

$$S_{(i-1)(n/3)+1} = 3/2, \qquad S_{(i-1)(n/3)+2} = \begin{pmatrix} 3/2 & -1 \\ -1 & 3/2 \end{pmatrix} = S_{i(n/3)}, \qquad 1 \le i \le n/3.$$

The sparse inverse approximation of $\det(T_3)$ is $\det(T_3) + 2/3$. It has no accurate digit because the relative error is $16/9$. The sparse inverse approximation of $\det(M)$ is $\sigma = (\det(T_3) + 2/3))^{n/3}$. For instance, when $n = 300$ then $\det(M) \approx 4 \cdot 10^{17}$ while the sparse inverse approximation gives $\sigma \approx 4 \cdot 10^{33}$.

Tridiagonal Toeplitz Matrices. A block diagonal approximation can be more accurate than a sparse inverse approximation if the dimension of the blocks is larger than 1. Let

$$T_n = \begin{pmatrix} 2 & -1 & & \\ -1 & 2 & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 2 \end{pmatrix}$$

be of order n; then $\det(T_n) = n + 1$. In the sparse inverse approximation (3) we fully exploit sparsity by choosing $S_1 = 2$ and $S_i = T_2$, $2 \le i \le n$; hence the approximation is $\sigma = 2 (3/2)^{n-1}$. When M_D in (1) consists of k equally sized blocks of dimension n/k then $\det(M_D) = \left(\det(T_{n/k})\right)^k = ((n/k) + 1)^k$. For a block size $n/k \ge 4$, $\det(M_D) \le \sigma$, so the block diagonal approximation is more accurate than the sparse inverse approximation.

2-D Laplacian. We show that for this matrix both, the block-diagonal and the sparse inverse approximations are accurate to at most one digit. The coefficient matrix from the centered finite difference discretization of Poisson's equation is a Hermitian positive-definite block tridiagonal matrix [11, 9.1.1]

$$M = \begin{pmatrix} T_m & -I_m & & \\ -I_m & T_m & \ddots & \\ & \ddots & \ddots & -I_m \\ & & -I_m & T_m \end{pmatrix}, \qquad \text{where} \quad T_m = \begin{pmatrix} 4 & -1 & & \\ -1 & 4 & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 4 \end{pmatrix}.$$

Here T_m is of order m, and M is of order $n = m^2$ (note that the matrix considered in [19, §5] equals $(n + 1)^2 M$). The exact determinant is [11, Theorem 9.1.2]

$$\det(M) = \prod_{i,j=1}^{m} 4\left(\sin\left(\frac{i\pi}{2(m+1)}\right)^2 + \sin\left(\frac{j\pi}{2(m+1)}\right)^2\right).$$

We compute the logarithm of this expression and compare it to the approximations. A block diagonal approximation (1) with $k = m$ gives $\det(M_D) = \det(T_m)^m$, where [12, §28.5]

$$\det(T_m) = \prod_{i=1}^{m}\left(4 + 2\cos\frac{i\pi}{m+1}\right).$$

If the matrices in the sparse inverse approximation (3) are

$$S_1 = 4, \qquad S_i = \begin{pmatrix} 4 & -1 \\ -1 & 4 \end{pmatrix}, \quad 2 \le i \le m+1, \qquad S_j = \begin{pmatrix} 4 & 0 & -1 \\ 0 & 4 & -1 \\ -1 & -1 & 4 \end{pmatrix}, \quad m+2 \le j \le n,$$

then $1/\sigma_1 = 4$, $1/\sigma_i = 15/4$, $2 \le i \le m + 1$, and $1/\sigma_j = 7/2$, $m + 2 \le j \le n$. Thus the sparse inverse approximation is $\sigma = 4(15/4)^m(7/2)^{n-m-1}$.

Table I lists errors for the block diagonal and sparse inverse approximations for $n = 900$, $n = 10000$ and $n = 40000$. Columns 3 and 4 represent the relative errors

$$|\ln(\det(M_D)) - \ln(\det(M))|/|\ln(\det(M))| \qquad \text{and} \qquad |\ln(\sigma) - \ln(\det(M))|/|\ln(\det(M))|,$$

while columns 5 and 6 represent the relative errors

$$|\det(M_D)^{1/n} - \det(M)^{1/n}|/|\det(M)^{1/n}| \qquad \text{and} \qquad |\sigma^{1/n} - \det(M)^{1/n}|/|\det(M)^{1/n}|.$$

We include the last two errors to allow a comparison with the approximation of $\det\left((n+1)^2 M\right)^{1/n}$ in [19, Table 5.1]. The table shows that all relative errors lie between 0.06 and 0.2. Hence both approximations, block diagonal and sparse inverse, are accurate to at most one significant digit. To estimate the tightness of the bound

$$|\ln(\det(M_D)) - \ln\det(M)| \le (-n\,|\ln(1-\rho)|)\,\rho$$

in Theorem 3, consider the case $n = 900$. Here $\rho(M_D^{-1} M_{\text{off}}) \approx .9898$ and $|\ln(1-\rho)| \approx 4.5845$. The true error is

$$|\ln(\det(M_D)) - \ln\det(M)| \approx 122.4966 \approx 26\ln(1-\rho)\,\rho.$$

The matrix $M_D^{-1} M_{\text{off}}$ has 26 eigenvalues with magnitude at least 0.9. Thus the pessimism of the bound comes from the factor n.

4. Application to Neutron Matter Simulations

In [16] we consider the quantum simulation of nuclear matter on a lattice, and in particular how to calculate the contribution of nucleon-nucleon-hole loops at non-zero nucleon density. The resulting method, called zone determinant expansion, is based on the sequence of

n	$\ln(\det(M))$	rel. error in $\ln(M_D)$	rel. error in $\ln(\sigma)$	rel error in $M_D^{1/n}$	rel. error in $\sigma^{1/n}$
900	1.0650e+03	0.1150	0.0607	0.1458	0.0745
10000	1.1717e+04	0.1246	0.0698	0.1572	0.0852
40000	4.6761e+04	0.1269	0.0719	0.1599	0.0877

Table I. Errors in the block diagonal approximation M_D and the sparse inverse approximation σ for the Laplacian.

approximations in Theorem 3. Here we illustrate that 3 iterations of the zone determinant expansion give an approximation accurate to 3 digits, and that the method uses less space than a determinant computation based on Gaussian elimination (with partial or complete pivoting).

In [16] we derive a particle interaction matrix M whose determinant $\det(M)$ is not positive, and complex in general. Hence stochastic methods such as hybrid Monte Carlo methods [7, 10, 20] do not give the correct sign or phase of $\det(M)$. This was the motivation for approximating $\ln(\det(M))$ via a zone determinant expansion, i.e. Theorem 3. Below we discuss the structure of M and a physically appropriate zone determinant expansion.

The particle interactions are considered on a 4-dimensional lattice (3 dimensions for space and one for time). Let the dimensions of the lattice be $L \times L \times L \times L_t$, where L_t represents the time direction. Also let the number of particles per lattice point be s. Then the interaction matrix M has dimension $n \times n$ where $n = L^3 L_t s$. We partition the lattice into separate spatial zones (or cubes) of dimension $m \times m \times m$ (constraints on m are discussed in [16]). Therefore particle interactions between any two zones are represented by matrix blocks of dimension $m^3 L_t s$. As a consequence, it makes sense to approximate $\det(M)$ by the product of principal minors associated with particle interactions inside spatial zones. Without loss of generality we assume that the lattice points are ordered such that the submatrix M_{ij} of order $m^3 L_t s$ represents particle interactions between zones i and j. With $k \equiv (L/m)^3$ this gives the partitioning $M = M_D + M_{\text{off}}$ in (1), where M_D represents particle interactions in the zone interiors, while M_{off} represents interactions among different zones. In [16] we explain that the spectral radius $\rho \equiv \rho(M_D^{-1} M_{\text{off}})$ can be reduced by increasing the dimension m of the spatial zones.

We illustrate the zone expansion on a small lattice simulation, where we can compare the approximations to the exact determinant. Specifically we consider the interactions between neutrons and neutral pions, on a $4^3 \times 4$ grid. The order of the interaction matrix M is $4^3 \times 4 \times 2 = 512$. Its properties are listed in Table II.

In the context of the particular application in [16], we can partition the lattice into zones with dimension $m = 1$. The resulting partitioning has blocks $M_{ij} \equiv M_{8(i-1)+1:8i,8(j-1)+1:j}$, $1 \le i, j \le 64$, of dimension $4 \times 2 = 8$. Thus $k = 64$ in the block diagonal approximation (1). Figure 2 shows the distribution of the 448 blocks with non-zero elements. Each diagonal block M_{ii} contains 24 non-zero elements, its sparsity structure is shown in Figure 2.

The zone partitioning is bipartite, i.e. $M_{ij} = 0$ for i and j both even or both odd, and $i \ne j$, $1 \le i, j \le k$. Therefore M_{off} is an odd checkerboard matrix. Figure 5 illustrates this
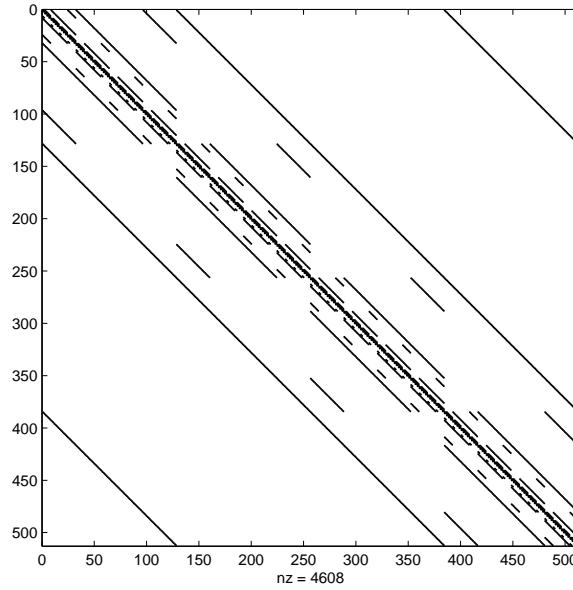
Figure 1. Sparsity structure of the interaction matrix M.

order	$n = 512$	
number of non-zeros	$9n$	see Figure 1
structure	complex non-Hermitian	see Figure 2
norm	$\|M\|_F \approx 49.5$	
condition number	$\|M\|_1\|M^{-1}\|_1 \approx 177$	condest$(\cdot)$ in MATLAB 6
non-normality	$\|M^*M - MM^*\|_F \approx 57$	
eigenvalues	complex	see Figure 3
determinant	$\det(M) = 8.5361 \cdot 10^{65} + 1.4168 \cdot 10^{64}\imath$	det$(\cdot)$ in Matlab 6
	$\ln(\det(M)) = 151.81 + 0.016599\imath$	

Table II. Properties of the interaction matrix M.

checkerboard pattern in the leading principal submatrix of order 32 of $M_D^{-1}M_{\text{off}}$. The sparsity structures of the matrices $M_D^{-1}M_{\text{off}}$ and $(M_D^{-1}M_{\text{off}})^2$ is shown in Figure 4. Because of the checkerboard structure Theorem 4 implies $\text{trace}((M_D^{-1}M_{\text{off}})^p) = 0$ for odd p, and $\delta_{p-1} = \delta_p$. Table III therefore contains only approximations of even order.

Table III shows errors in the approximations δ_j and Δ_j for approximations up to order 8. Columns 2, 3 and 4 represent the absolute errors

$$|\Re(\ln(\det(M))) - \Re(\delta_j)|, \qquad |\Im(\ln(\det(M))) - \Im(\delta_j)|, \qquad |\ln(\det(M)) - \delta_j|.$$

Columns 6 and 7 represent the relative errors

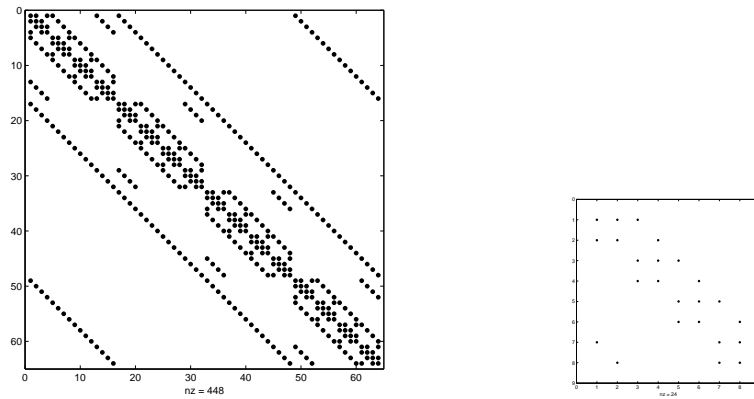$$|\ln(\det(M)) - \delta_j|/|\delta_j| \qquad \text{and} \qquad |\det(M) - \Delta_j|/|\Delta_j|.$$

Figure 2. Non-zero 8×8 blocks in the interaction matrix M, and sparsity structure of a single 8×8 diagonal block.
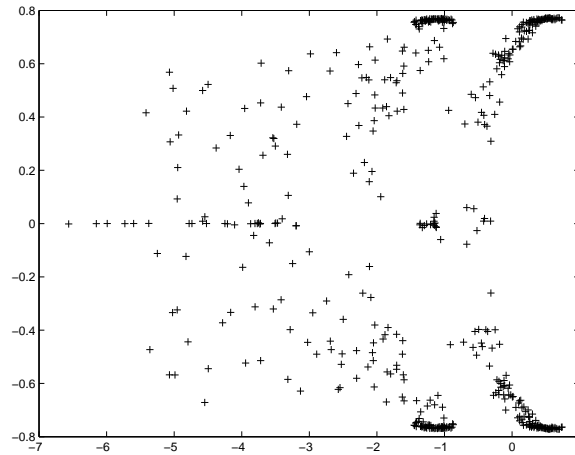

Figure 3. Eigenvalue distribution of the interaction matrix M.

j	abs. error in $\Re(\delta_j)$	abs. error in $\Im(\delta_j)$	abs. error in δ_j	ρ^j	rel. error in δ_j	rel. error in Δ_j
0	5.1000	0.0017	5.1000		0.0348	163.0282
2	0.4817	0.0025	0.4817	0.4374	0.0032	0.3823
4	0.0909	0.0016	0.0909	0.1913	0.0006	0.0951
6	0.0225	0.0008	0.0226	0.0837	0.0001	0.0223
8	0.00665	0.0003	0.0066	0.0366	0.00004	0.0066

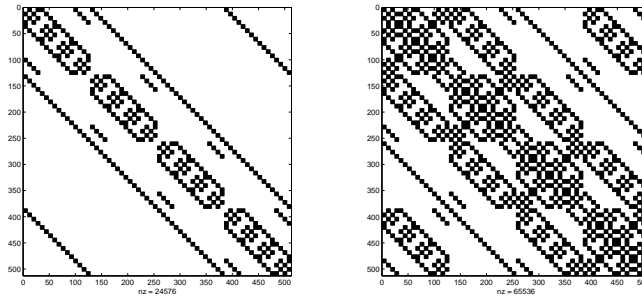Table III. Errors in the approximations δ_j and Δ_j for the interaction matrix M.

Figure 4. Sparsity structure of the matrices $M_D^{-1} M_{\text{off}}$ and $(M_D^{-1} M_{\text{off}})^2$.
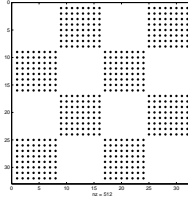

Figure 5. Sparsity structure of the leading principal submatrix of order 32 of $M_D^{-1} M_{\text{off}}$.

The spectral radius $\rho \equiv \rho(M_D^{-1} M_{\text{off}}) \approx .6613$, and the constant in the error bounds of Theorems 2 and 3 is $c \approx 554$.

Table III illustrates that $|\ln(\det(M)) - \delta_j| \approx \rho^j$, i.e. the absolute errors in the logarithm are almost proportional to the powers of the spectral radius of $M_D^{-1} M_{\text{off}}$. In this case the constant c is too pessimistic, because many eigenvalues of $M_D^{-1} M_{\text{off}}$ have magnitude much less than ρ. For instance, 160 eigenvalues of $M_D^{-1} M_{\text{off}}$ have magnitude 10^{-15}. The imaginary parts of the logarithms appear to converge faster than the real parts. The block diagonal approximation $\delta_0 \equiv \ln(\det(M_D))$ for $\ln(\det(M))$ has an accuracy of 2 digits. Two more iterations give an approximation δ_2 that is accurate to 3 digits.

We briefly compare the computation of δ_0 and δ_2 to a determinant computation by Gaussian elimination of M. Gaussian elimination with complete pivoting gives $PMQ = LU$, where P and Q are permutation matrices, L is unit lower triangular and U is upper triangular. Figure 6, which shows the sparsity structure of the matrices PMQ, L and U, illustrates that Gaussian elimination with complete pivoting completely destroys the sparsity structure of M. The matrices L and U together have about $162n$ non-zeros, compared to $9n$ in M. In contrast, the determinant expansion requires no significant additional space for δ_0; and $48n$ non-zeros for $M_D^{-1} M_{\text{off}}$ and n non-zeros for the trace of $(M_D^{-1} M_{\text{off}})^2$. That's $(48 + 1)n = 49n$ non-zeros, about one third of the non-zeros produced by Gaussian elimination with complete pivoting. Gaussian elimination with partial pivoting essentially preserves the sparsity structure of M but produces $342n$ non-zeros.
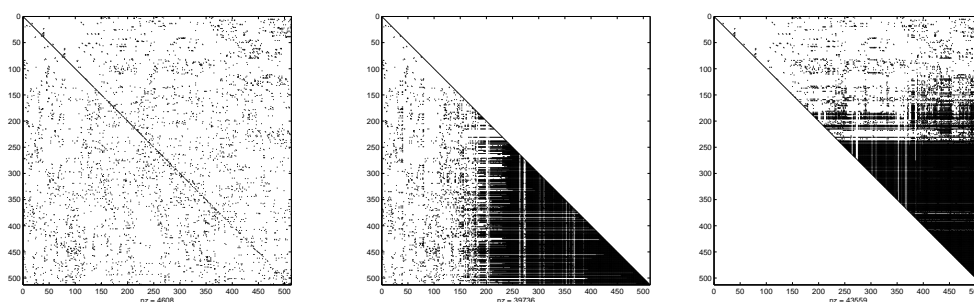
Figure 6. Sparsity structure of the matrices PMQ, L and U from the LU decomposition (with complete pivoting) of M.

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