Several Methods for Computing Determinants of Large Sparse Matrices

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Overview

Large sparse complex matrix M of order n

Want: $\ln\det(M)$ or $\det(M)^{1/n}$

- Block-Diagonal Approximations
- Zone Determinant Expansion
- Principal Minors of Inverses
- Sparse Inverse Approximations
- Properties
- Numerical Experiments

Literature

Sparse Hermitian positive-definite matrices

- Sparse Approximate Inverses
  Reusken 2002
- Monte Carlo
  Reusken 2002
- Hybrid Monte Carlo
  Duane, Kennedy, Pendelton, Roweth 1987
  Gottlieb, Liu, Toussaint, Renke, Sugar 1987
  Scalettar, Scalapino, Sugar 1986
- Gaussian Quadrature
  Bai & Golub 1997

Block-Diagonal Approximations

$$\begin{pmatrix} X & X & X & X & X \\ X & X & X & X & X \\ X & X & X & X & X \\ X & X & X & X & X \\ X & X & X & X & X \end{pmatrix} = \begin{pmatrix} X & X & & & \\ X & X & & & \\ & & X & & \\ & & & X & X \\ & & & X & X \end{pmatrix} + \begin{pmatrix} & & X & X & X \\ & & X & X & X \\ X & X & & X & X \\ X & X & X & & \\ X & X & X & & \end{pmatrix}$$

$$M = D + O$$

Is $\det(D)$ a good approximation for $\det(M)$?

Block-Diagonal Approximations

If $M = D + O$ is Hermitian positive-definite then

- Hadamard-Fischer: $\det(M) \leq \det(D)$
- Relative error:

$$0 < \frac{\det(D) - \det(M)}{\det(D)} \leq c\rho\, e^{c\rho}$$

where $\rho \equiv \max_j |\lambda_j(D^{-1}O)|$

$c \equiv -n \ln(1-\rho)$, $\quad n$ is order of M

Block-Diagonal Approximations

$M = D + O$ with $\rho \equiv \max_j |\lambda_j(D^{-1}O)| < 1$

$$\frac{|\det(D) - \det(M)|}{|\det(D)|} \leq c\rho\, e^{c\rho}$$

where $c \equiv -n \ln (1-\rho)$, n is order of M

Block-diagonal approximation $\det(D)$ good

if eigenvalues of $D^{-1}O$ close to zero

Diagonal Approximation

M strictly row diagonally dominant

$$\frac{\left|\prod m_{ii} - \det(M)\right|}{\left|\prod m_{ii}\right|} \leq c\rho\, e^{c\rho}$$

where

$$\rho \leq \max_i \sum_{j \neq i} \left| \frac{m_{ij}}{m_{ii}} \right|$$

Product of diagonal elements good approximation if M strongly diagonally dominant

Zone Determinant Expansion

[Lee & Il 2003]

If D non-singular and $\rho(D^{-1}O) < 1$ then

$$\det(M) = \det(D+O) = \det(D)\,\underbrace{\det(I + D^{-1}O)}_{\text{expand}}$$

$$\begin{aligned}\det(I + D^{-1}O) &= \exp\left(\mathrm{trace}(\log(I + D^{-1}O))\right)\\ &= \exp\left(\sum_{i=1}^{\infty} \frac{(-1)^i}{i}\,\mathrm{trace}((D^{-1}O)^i)\right)\end{aligned}$$

Zone Determinant Expansion

$M = D + O$ with $\rho \equiv \max_j |\lambda_j(D^{-1}O)| < 1$

$$Z_m \equiv \ln \det(D) + \sum_{i=1}^{m} \frac{(-1)^i}{i} \operatorname{trace}((D^{-1}O)^i)$$

Bound for Logarithm:

$$|\ln(\det(M)) - Z_m| \leq c\rho^m$$

where $c \equiv -n \ln(1 - \rho)$

Zone Determinant Expansion

$M = D + O$ with $\rho \equiv \max_j |\lambda_j(D^{-1}O)| < 1$

$$Z_m \equiv \ln \det(D) + \sum_{i=1}^{m} \frac{(-1)^i}{i} \operatorname{trace}((D^{-1}O)^i)$$

$$\frac{|\det(M) - e^{Z_m}|}{|e^{Z_m}|} \leq c\rho^m \, e^{c\rho^m}$$

where $c \equiv -n \ln(1 - \rho)$

Summary: Zone Determinant Exp.

$M = D + O$ with D block diagonal

$$\rho \equiv \max_j |\lambda_j(D^{-1}O)| < 1$$

$$Z_m \equiv \ln\det(D) + \sum_{i=1}^{m} \frac{(-1)^i}{i} \mathrm{trace}((D^{-1}O)^i)$$

$$Z_0 = \ln\det(D)$$ block diagonal approximation

$Z_m \approx \ln\det(M)$ $\quad e^{Z_m} \approx \det(M)$ $\quad$ Error $\sim \rho^m e^{\rho^m}$

Principal Minors of Inverses

M Hermitian positive-definite, of order n

$$M = \begin{pmatrix} M_{n-1} & * \\ * & * \end{pmatrix} \qquad M^{-1} = \begin{pmatrix} * & * \\ * & \sigma \end{pmatrix}$$

$$\det(M) = \frac{1}{\sigma} \det(M_{n-1})$$

Cholesky: $M = LL^*$ $\qquad \dfrac{1}{\sigma} = L_{nn}^2$

Cholesky Factorization

$$M = LL^* = \begin{pmatrix} L_{11} & & \\ * & L_{22} & \\ * & * & L_{33} \end{pmatrix} \begin{pmatrix} L_{11} & * & * \\ & L_{22} & * \\ & & L_{33} \end{pmatrix}$$

$$M^{-1} = L^{-*}L^{-1} = \begin{pmatrix} \frac{1}{L_{11}} & * & * \\ & \frac{1}{L_{22}} & * \\ & & \frac{1}{L_{33}} \end{pmatrix} \begin{pmatrix} \frac{1}{L_{11}} & & \\ * & \frac{1}{L_{22}} & \\ * & * & \frac{1}{L_{33}} \end{pmatrix}$$

$$\sigma = (M^{-1})_{33} = \left(\frac{1}{L_{33}}\right)^2$$

Principal Minors of Inverses

$$M = \begin{pmatrix} M_{n-1} & * \\ * & * \end{pmatrix} \qquad M^{-1} = \begin{pmatrix} * & * \\ * & \sigma_n \end{pmatrix}$$

$$\det(M) = \det(M_{n-1})/\sigma_n$$

$$M_{n-1} = \begin{pmatrix} M_{n-2} & * \\ * & * \end{pmatrix} \qquad M_{n-1}^{-1} = \begin{pmatrix} * & * \\ * & \sigma_{n-1} \end{pmatrix}$$

$$\det(M_{n-1}) = \det(M_{n-2})/\sigma_{n-1}$$

$$\det(M) = \frac{1}{\sigma_n}\frac{1}{\sigma_{n-1}} \det(M_{n-2})$$

Summary: Principal Minors

M Hermitian positive-definite, of order n

$$M = \begin{array}{c c} & \begin{array}{cc} i & n-i \end{array} \\ \begin{array}{c} i \\ n-i \end{array} & \begin{pmatrix} M_i & * \\ * & * \end{pmatrix} \end{array} \qquad M_i^{-1} = \begin{pmatrix} * & * \\ * & \sigma_i \end{pmatrix}$$

$$\det(M) = \prod_{i=1}^{n} \frac{1}{\sigma_i}$$

Cholesky: $M_i = L_i L_i^*$ $\qquad \dfrac{1}{\sigma_i} = ((L_i)_{ii})^2$

Sparse Inverse Approximations

[Reusken 2002], [Lee & Il 2004]

Hermitian positive-definite M

- Exact: $\det(M) = \prod \frac{1}{\sigma_i}$
  σ_i last diagonal element of M_i^{-1}
  $M_i = M(1:i, 1:i)$
- Approximate: $\Delta = \prod \frac{1}{\sigma_i}$
  σ_i last diagonal element of S_i^{-1}
  S_i principal submatrix of M_i

Diagonal Approximation

$$M = \begin{pmatrix} M_{11} & M_{12} & M_{13} & M_{14} & M_{15} & M_{16} \\ M_{21} & M_{22} & M_{23} & M_{24} & M_{25} & M_{26} \\ M_{31} & M_{32} & M_{33} & M_{34} & M_{35} & M_{36} \\ M_{41} & M_{42} & M_{43} & M_{44} & M_{54} & M_{46} \\ M_{51} & M_{52} & M_{53} & M_{54} & M_{55} & M_{56} \\ M_{61} & M_{62} & M_{63} & M_{64} & M_{65} & m_{66} \end{pmatrix}$$

$$S_i = M_{ii} \qquad \det(M) \approx \prod_i M_{ii}$$

Block Diagonal Approximation

$i = 1$:

$$M = \begin{pmatrix} M_{11} & M_{12} & M_{13} & M_{14} & M_{15} & M_{16} \\ M_{21} & M_{22} & M_{23} & M_{24} & M_{25} & M_{26} \\ M_{31} & M_{32} & M_{33} & M_{34} & M_{35} & M_{36} \\ M_{41} & M_{42} & M_{43} & M_{44} & M_{54} & M_{46} \\ M_{51} & M_{52} & M_{53} & M_{54} & M_{55} & M_{56} \\ M_{61} & M_{62} & M_{63} & M_{64} & M_{65} & M_{66} \end{pmatrix}$$

$$S_1 = M_{11} \qquad \sigma_1 = 1/M_{11}$$

Block Diagonal Approximation

$i = 2$:

$$M = \begin{pmatrix} M_{11} & M_{12} & M_{13} & M_{14} & M_{15} & M_{16} \\ M_{21} & M_{22} & M_{23} & M_{24} & M_{25} & M_{26} \\ M_{31} & M_{32} & M_{33} & M_{34} & M_{35} & M_{36} \\ M_{41} & M_{42} & M_{43} & M_{44} & M_{54} & M_{46} \\ M_{51} & M_{52} & M_{53} & M_{54} & M_{55} & M_{56} \\ M_{61} & M_{62} & M_{63} & M_{64} & M_{65} & M_{66} \end{pmatrix}$$

$$S_2 = M_{22} \qquad \sigma_2 = 1/M_{22}$$

Block Diagonal Approximation

$i = 3$:

$$M = \begin{pmatrix} {\color{blue}M_{11}} & M_{12} & M_{13} & M_{14} & M_{15} & M_{16} \\ M_{21} & {\color{red}M_{22}} & {\color{red}M_{23}} & M_{24} & M_{25} & M_{26} \\ M_{31} & {\color{red}M_{32}} & {\color{red}M_{33}} & M_{34} & M_{35} & M_{36} \\ M_{41} & M_{42} & M_{43} & M_{44} & M_{54} & M_{46} \\ M_{51} & M_{52} & M_{53} & M_{54} & M_{55} & M_{56} \\ M_{61} & M_{62} & M_{63} & M_{64} & M_{65} & M_{66} \end{pmatrix}$$

$$S_3 = \begin{pmatrix} M_{22} & M_{23} \\ M_{32} & M_{33} \end{pmatrix} \qquad \sigma_3 = (S_3^{-1})_{22}$$

Block Diagonal Approximation

$i = 4$:

$$M = \begin{pmatrix} M_{11} & M_{12} & M_{13} & M_{14} & M_{15} & M_{16} \\ M_{21} & M_{22} & M_{23} & M_{24} & M_{25} & M_{26} \\ M_{31} & M_{32} & M_{33} & M_{34} & M_{35} & M_{36} \\ M_{41} & M_{42} & M_{43} & M_{44} & M_{54} & M_{46} \\ M_{51} & M_{52} & M_{53} & M_{54} & M_{55} & M_{56} \\ M_{61} & M_{62} & M_{63} & M_{64} & M_{65} & M_{66} \end{pmatrix}$$

$$S_4 = \begin{pmatrix} M_{22} & M_{23} & M_{24} \\ M_{32} & M_{33} & M_{34} \\ M_{42} & M_{43} & M_{44} \end{pmatrix} \qquad \sigma_4 = (S_4^{-1})_{33}$$

Block Diagonal Approximation

$i = 5$:

$$M = \begin{pmatrix} M_{11} & M_{12} & M_{13} & M_{14} & M_{15} & M_{16} \\ M_{21} & M_{22} & M_{23} & M_{24} & M_{25} & M_{26} \\ M_{31} & M_{32} & M_{33} & M_{34} & M_{35} & M_{36} \\ M_{41} & M_{42} & M_{43} & M_{44} & M_{54} & M_{46} \\ M_{51} & M_{52} & M_{53} & M_{54} & M_{55} & M_{56} \\ M_{61} & M_{62} & M_{63} & M_{64} & M_{65} & M_{66} \end{pmatrix}$$

$$S_5 = M_{55} \qquad \sigma_5 = 1/M_{55}$$

Block Diagonal Approximation

$i = 6$:

$$M = \begin{pmatrix} M_{11} & M_{12} & M_{13} & M_{14} & M_{15} & M_{16} \\ M_{21} & M_{22} & M_{23} & M_{24} & M_{25} & M_{26} \\ M_{31} & M_{32} & M_{33} & M_{34} & M_{35} & M_{36} \\ M_{41} & M_{42} & M_{43} & M_{44} & M_{54} & M_{46} \\ M_{51} & M_{52} & M_{53} & M_{54} & M_{55} & M_{56} \\ M_{61} & M_{62} & M_{63} & M_{64} & M_{65} & M_{66} \end{pmatrix}$$

$$S_6 = \begin{pmatrix} M_{55} & M_{56} \\ M_{65} & M_{66} \end{pmatrix} \qquad \sigma_6 = (S_6^{-1})_{22}$$

Observing Sparsity

$$T_3 = \begin{pmatrix} 3/2 & -1 & \\ -1 & 3/2 & -1 \\ & -1 & 3/2 \end{pmatrix} \qquad \det(T_3) = \frac{3}{8}$$

$$\begin{pmatrix} 3/2 & -1 & \\ -1 & 3/2 & -1 \\ & -1 & 3/2 \end{pmatrix} \quad \begin{pmatrix} 3/2 & -1 & \\ -1 & 3/2 & -1 \\ & -1 & 3/2 \end{pmatrix} \quad \begin{pmatrix} 3/2 & -1 & \\ -1 & 3/2 & -1 \\ & -1 & 3/2 \end{pmatrix}$$

$$\Delta = \frac{3}{2}\left(\frac{5}{6}\right)^2 = \det(T_3) + \frac{2}{3}$$

Summary: Sparse Inverse Approx.

$$M = \begin{pmatrix} M_i & * \\ * & * \end{pmatrix}$$ Hermitian positive-definite

For $i = 1 \dots n$

- S_i is principal submatrix of M_i (must contain row and column i of M_i)
- σ_i is trailing diagonal element of S_i^{-1}

$$\Delta = \prod_{i=1}^{n} \frac{1}{\sigma_i}$$

Properties

M Hermitian positive-definite

- Any sparse inverse approximation $\Delta = \prod \frac{1}{\sigma_i}$ is an upper bound for $\det(M)$

$$\det(M) \leq \Delta$$

- Monotonicity

$$S_{n\times n} = \begin{pmatrix} * & * \\ * & S_{m\times m} \end{pmatrix} \qquad \frac{1}{(S_{n\times n}^{-1})_{nn}} \leq \frac{1}{(S_{m\times m}^{-1})_{mm}}$$

Properties

M Hermitian positive-definite

- Larger submatrix $\Rightarrow$ better approximation

$$M = \begin{pmatrix} * & * & * \\ * & * & * \\ * & * & \hat{S}_n \end{pmatrix} \qquad S_n \equiv \begin{pmatrix} * & * \\ * & \hat{S}_n \end{pmatrix}$$

$\hat{\Delta}$ uses last diagonal element of $\hat{S}_n^{-1}$

Δ uses last diagonal element of S_n^{-1}

$$\det(M) \leq \Delta \leq \hat{\Delta}$$

Properties

$M = D + O$ Hermitian positive-definite

- Any sparse inverse approximation $\Delta = \prod \frac{1}{\sigma_i}$ at least as accurate as diagonal approximation

$$\det(M) \leq \Delta \leq \prod_i M_{ii}$$

- Sparse inverse approximations can be less accurate than a block diagonal approximation

$$\det(M) \leq \det(D) \leq \Delta \quad \text{is possible}$$

Tridiagonal Toeplitz Matrices

$$T_n = \begin{pmatrix} 2 & -1 & & \\ -1 & 2 & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 2 \end{pmatrix} \qquad \det(T_n) = n + 1$$

- Sparse Inverse: $S_1 = 2$, $S_i = T_2$, $\Delta = 2\ \left(\frac{3}{2}\right)^{n-1}$
- Blockdiagonal: $T_n = D + O$, $\det(D) = \left(\frac{n}{k} + 1\right)^k$
- Block diagonal better for blocks of order ≥ 4

$$\det(M) \leq \det(D) \leq \Delta \qquad \text{for} \quad n/k \geq 4$$

2D Laplacian

$$M = \begin{pmatrix} T_m & -I_m & & \\ -I_m & T_m & \ddots & \\ & \ddots & \ddots & -I_m \\ & & -I_m & T_m \end{pmatrix} \qquad m^2 \times m^2$$

$$T_m = \begin{pmatrix} 4 & -1 & & \\ -1 & 4 & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 4 \end{pmatrix}$$

2D Laplacian ($n = 9$)

$$
\begin{matrix}
4 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
-1 & 4 & -1 & 0 & -1 & 0 & 0 & 0 & 0 \\
0 & -1 & 4 & 0 & 0 & -1 & 0 & 0 & 0 \\
-1 & 0 & 0 & 4 & -1 & 0 & -1 & 0 & 0 \\
0 & -1 & 0 & -1 & 4 & -1 & 0 & -1 & 0 \\
0 & 0 & -1 & 0 & -1 & 4 & 0 & 0 & -1
\end{matrix}
$$

Sparse inverse approximation: $i = 1$

2D Laplacian ($n = 9$)

$$\begin{matrix} 4 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 4 & -1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 4 & 0 & 0 & -1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 4 & -1 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & -1 & 4 & -1 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & -1 & 4 & 0 & 0 & -1 \end{matrix}$$

Sparse inverse approximation: $i = 2$

2D Laplacian ($n = 9$)

$$
\begin{matrix}
4 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
-1 & 4 & -1 & 0 & -1 & 0 & 0 & 0 & 0 \\
0 & -1 & 4 & 0 & 0 & -1 & 0 & 0 & 0 \\
-1 & 0 & 0 & 4 & -1 & 0 & -1 & 0 & 0 \\
0 & -1 & 0 & -1 & 4 & -1 & 0 & -1 & 0 \\
0 & 0 & -1 & 0 & -1 & 4 & 0 & 0 & -1
\end{matrix}
$$

Sparse inverse approximation: $i = 3$

2D Laplacian ($n = 9$)

$$\begin{matrix} 4 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 4 & -1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 4 & 0 & 0 & -1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 4 & -1 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & -1 & 4 & -1 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & -1 & 4 & 0 & 0 & -1 \end{matrix}$$

Sparse inverse approximation: $i = 4$

2D Laplacian ($n = 9$)

$$\begin{array}{rrrrrrrrr} 4 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 4 & -1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 4 & 0 & 0 & -1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 4 & -1 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & -1 & 4 & -1 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & -1 & 4 & 0 & 0 & -1 \end{array}$$

Sparse inverse approximation: $i = 5$

2D Laplacian ($n = 9$)

$$\begin{matrix} 4 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 4 & -1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 4 & 0 & 0 & -1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 4 & -1 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & -1 & 4 & -1 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & -1 & 4 & 0 & 0 & -1 \end{matrix}$$

Sparse inverse approximation: $i = 6$

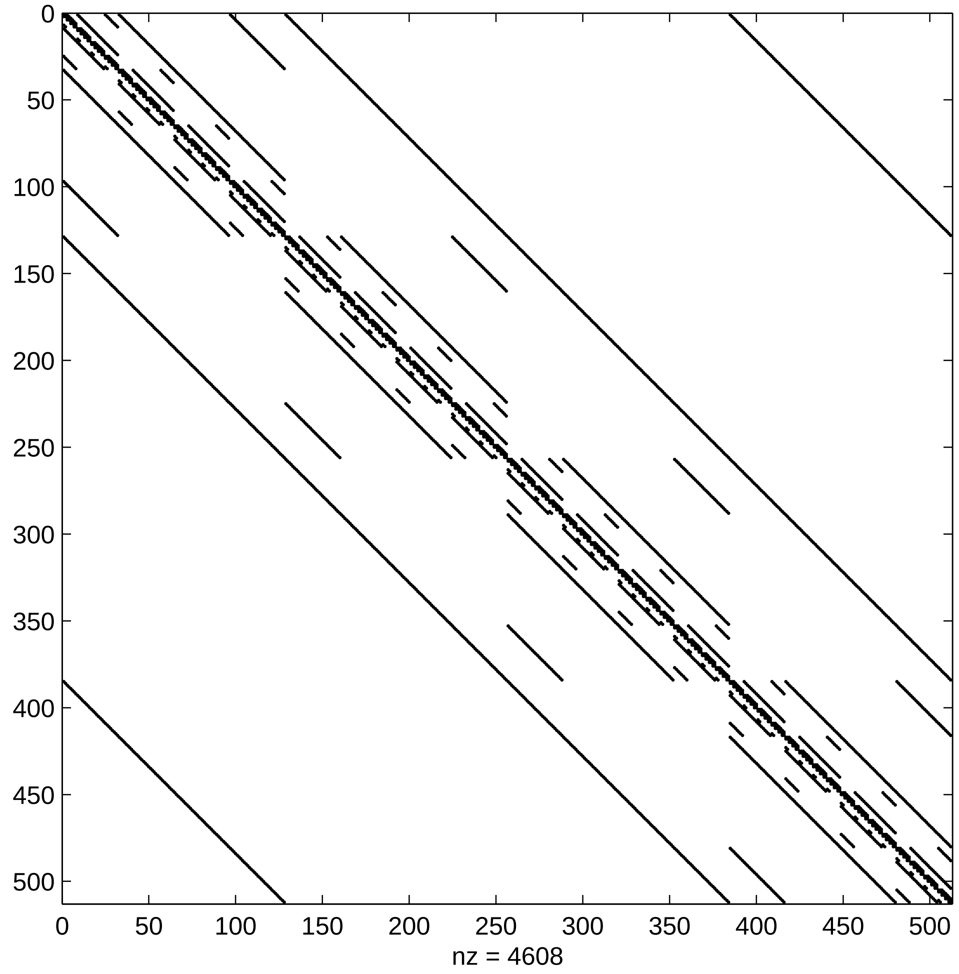
Relative Errors

Block diagonal D, blocks of order m
Sparse inverse approximation Δ

n	$\ln\det(M)$	error $\ln(D)$	error $\ln(\Delta)$	error $D^{1/n}$	error $\Delta^{1/n}$
900	1.1e+3	0.11	0.06	0.15	0.07
10000	1.2e+4	0.12	0.07	0.16	0.09
40000	4.7e+4	0.13	0.07	0.16	0.09

Accuracy for both methods: 1 digit

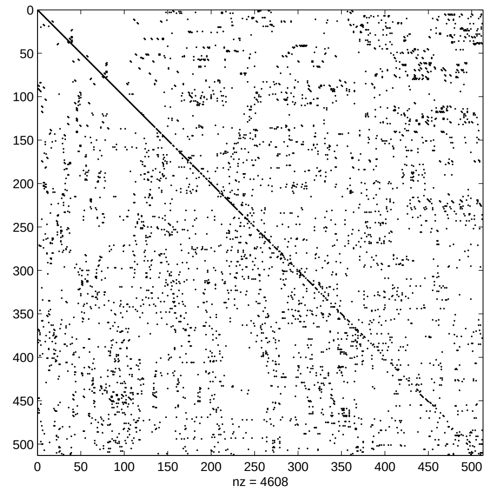
Neutron Matter Simulations

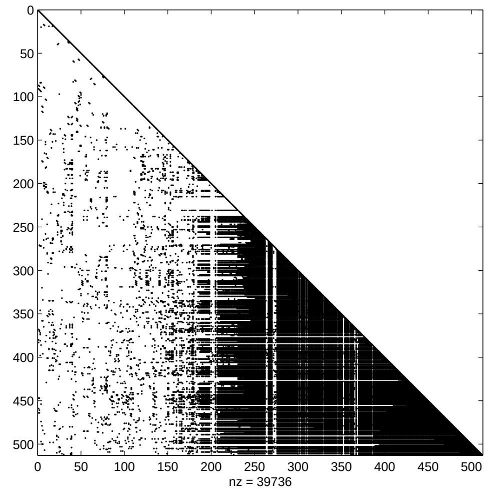


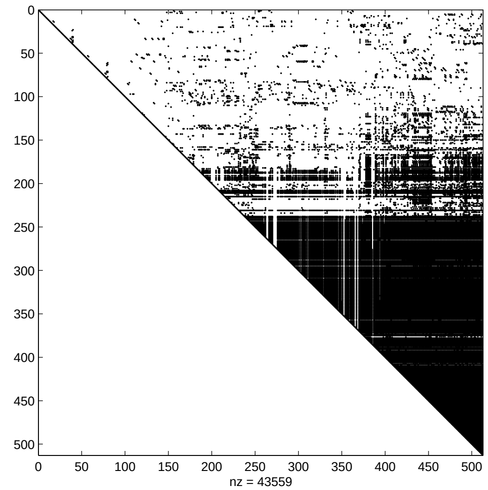
Interaction matrix M

LU Decomposition

With complete pivoting



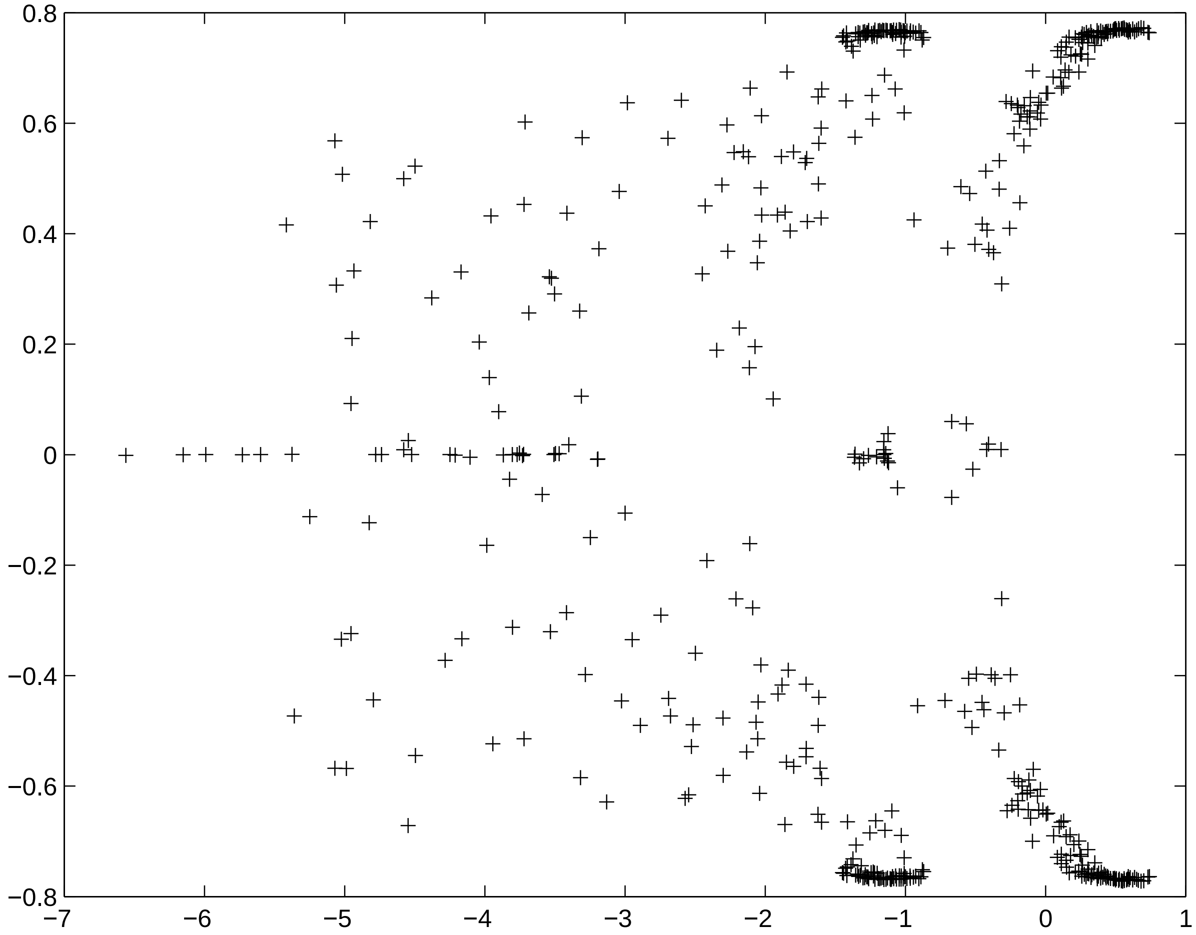




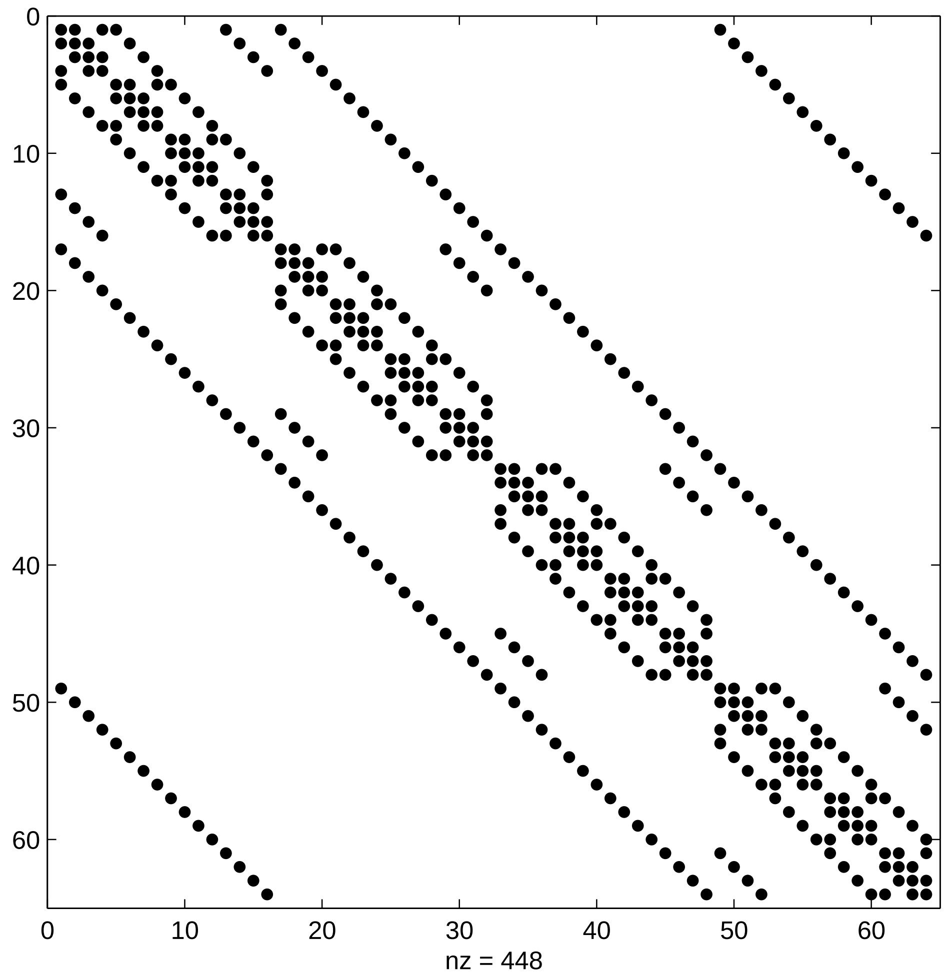
Interaction Matrix M

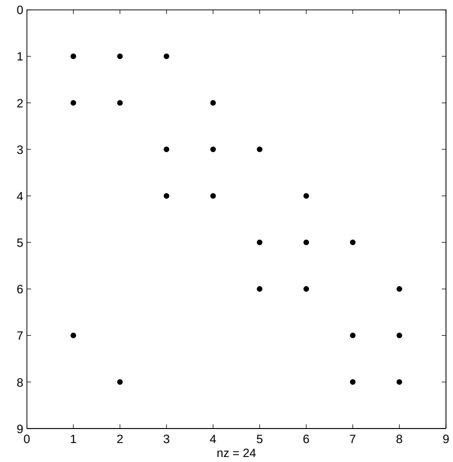
order	$n = 512$
# non-zeros	$9n$
structure	complex non-Hermitian
norm	$\|M\|_F \approx 49.5$
condition number	$\|M\|_1 \|M^{-1}\|_1 \approx 177$
non-normality	$\|M^*M - MM^*\|_F \approx 57$
eigenvalues	complex
determinant	$\det(M) = 8.5 \cdot 10^{65} + 1.4 \cdot 10^{64}\imath$
	$\ln(\det(M)) = 151.8 + 0.02\imath$

Eigenvalues of M



Non-Zero 8×8 blocks of M





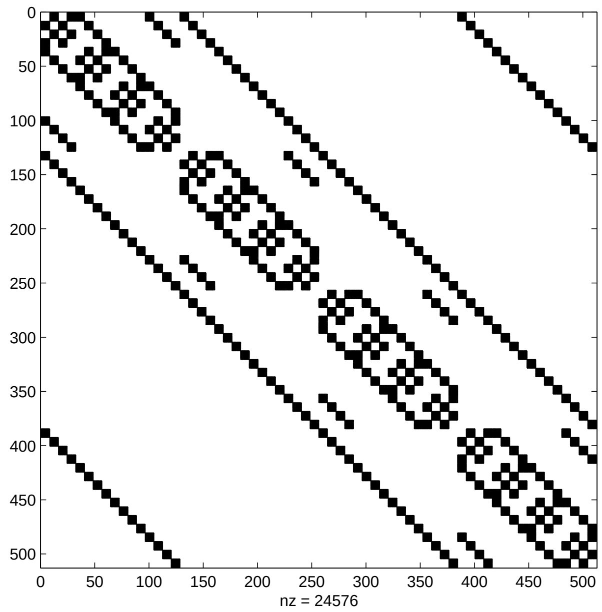
448 non-zero blocks, 24 non-zero entries/block

Zone Determinant Expansion

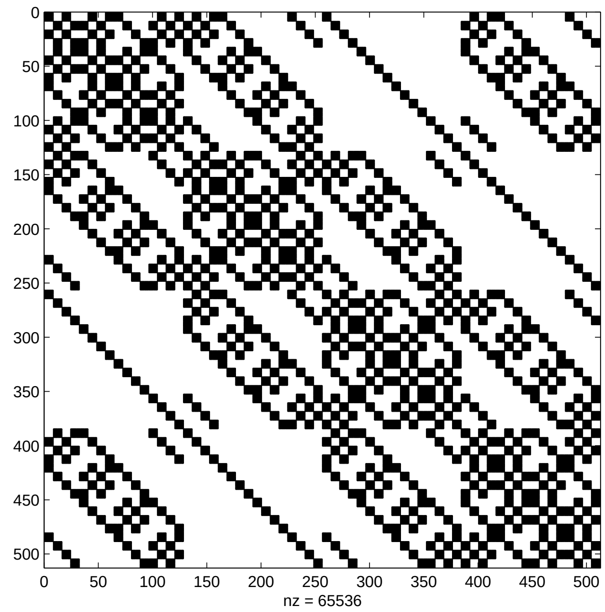
$$M = D + O$$

- D block diagonal, blocks of size 8×8
- $D^{-1}O$ is checkerboard matrix
  $\mathrm{trace}(D^{-1}O)^j = 0 \qquad$ for odd j
- Spectral radius $\rho\left(D^{-1}O\right) \approx .66$
- Expansions:
  $Z_0 = \ln\det(D)$
  $Z_j = \ln\det(D) + \sum_{i=1}^{j} \frac{(-1)^i}{i}\,\mathrm{trace}((D^{-1}O)^i)$

$D^{-1}O$ **And** $(D^{-1}O)^2$



0
50
100
150
200
250
300
350
400
450
500
nz = 24576



0
50
100
150
200
250
300
350
400
450
500
nz = 65536

Accuracy

j	error $\Re(Z_j)$	error $\Im(Z_j)$	error Z_j	ρ^j	error e^{Z_j}
0	5.100	0.0017	5.100		163.0282
2	0.482	0.0025	0.482	0.44	0.3823
4	0.091	0.0016	0.091	0.19	0.0951
6	0.023	0.0008	0.023	0.08	0.0223
8	0.007	0.0003	0.007	0.04	0.0066

Absolute error for $Z_j \approx \ln\det(M)$

Relative error for $e^{Z_j} \approx \det(M)$

Zone Determinant Expansion

$M = D + O$, $\rho = \rho(D^{-1}O)$

- Error in logarithm: $|\ln\det(M) - Z_j| < \rho^j$
- Accuracy:
  1 digit for $Z_0 = \ln\det(D)$, 3 digits for Z_2
  1 digit for $e^{Z_2} \approx \det(M)$
- Storage:
  Z_2: $49n$ non-zeros
  GE with complete pivoting: 162 non-zeros
  GE with partial pivoting: 342 non-zeros

Summary

- Two methods for computing determinants:
  Zone determinant expansion
  Sparse inverse approximation
- Sparse inverse approximation:
  only Hermitian positive-definite matrices
- Zone determinant expansion:
  relative error bounds
  efficient for neutron matter simulations
- 2D Laplacian:
  Block diagonal approximation competitive with sparse inverse approximation