Determinant Approximations

Ilse Ipsen

North Carolina State University

Joint Work with Dean Lee (Physics)

Overview

- Existing methods and determinant inequalities
- Our idea
- Diagonal approximations
- Sequence of higher order approximations
- Zone determinant expansions
- Extension of existing determinant inequalities

Application

Quantum simulation of nuclear matter on lattice
Determinant $\longrightarrow$ nucleon interactions

Computing determinants

- Monte Carlo: not accurate
- Gaussian elimination: too expensive
- Sparse approximate inverses: too limited
- Diagonal approximations

Fischer's Inequality

If M is Hermitian positive definite

$$M = \begin{pmatrix} M_{11} & * \\ * & M_{22} \end{pmatrix}$$

then

$$0 \leq \det(M) \leq \det(M_{11}) \det(M_{22})$$

Hadamard's Inequality

If M is Hermitian positive definite

$$M = \begin{pmatrix} m_{11} & * & * & * \\ * & m_{22} & * & * \\ * & * & m_{33} & * \\ * & * & * & \ddots \end{pmatrix}$$

then

$$0 \le \det(M) \le \prod_j m_{jj}$$

Diagonal Approximations

- Upper bounds on determinant
- For Hermitian positive-definite matrices
- (Almost) no error bounds
- Not for indefinite or non-Hermitian matrices

$$M = \begin{pmatrix} 1 & \frac{\imath}{2} \\ \frac{\imath}{2} & 1 \end{pmatrix}, \qquad \imath \equiv \sqrt{-1}$$

$$\det(M) = 1.25 > 1 = m_{11} m_{22}$$

Rescuing Diagonal Approximations

- Write $\det(M) = \exp(\mathrm{trace}(\log(M)))$
- Expand
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Why Does This Make Sense?

$$M = \begin{pmatrix} \alpha & \\ & \beta \end{pmatrix}$$

$$\begin{aligned} \det(M) &= \alpha \cdot \beta \\ &= e^{\ln \alpha} \cdot e^{\ln \beta} = e^{\ln \alpha + \ln \beta} \\ &= e^{\operatorname{trace}(\log(M))} \end{aligned}$$

$$\log(M) = \begin{pmatrix} \ln \alpha & \\ & \ln \beta \end{pmatrix}$$

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- Set $\log(X) := W$

$$\det(X) = \exp(\mathrm{trace}(\log(X)))$$

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$\det(M) = \det(D) \cdot e^{\alpha}$, where

$$\alpha = \operatorname{trace}(A) - \frac{1}{2}\operatorname{trace}(A^2) + \frac{1}{3}\operatorname{trace}(A^3) - \cdots$$

First Approximation

$\Delta \equiv \det(D) \cdot \exp(\mathrm{trace}(A))$

$\det(M) = \Delta \cdot e^z$, where

$$z = -\frac{1}{2}\,\mathrm{trace}(A^2) + \frac{1}{3}\,\mathrm{trace}(A^3) - \cdots$$

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Relative error

$$\left|\frac{\det(M) - \Delta}{\Delta}\right| = |1 - e^z|$$

First Approximation

$M = D + O$ of order n

$$\Delta \equiv \det(D) \cdot \exp(\mathrm{trace}(D^{-1}O))$$

If $\rho \equiv \rho(D^{-1}O) < 1$ then

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

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

Diagonal Approximations

$M = D + O$ of order n

$$D = \begin{pmatrix} * & & \\ & * & \\ & & * \end{pmatrix} \qquad O = \begin{pmatrix} 0 & * & * \\ * & 0 & * \\ * & * & 0 \end{pmatrix}$$

If $\rho \equiv \rho(D^{-1}O) < 1$ then

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

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

"Diagonally Dominant" Matrices

$M = D + O$ of order n

$$D = \begin{pmatrix} * & & \\ & * & \\ & & * \end{pmatrix} \qquad O = \begin{pmatrix} 0 & * & * \\ * & 0 & * \\ * & * & 0 \end{pmatrix}$$

If $\rho \equiv \rho(D^{-1}O) < \frac{1}{n+1}$ then

$$\left| \frac{\det(M) - \det(D)}{\det(D)} \right| \leq \frac{2}{1-\rho}\, \rho^2$$

Higher Order Approximations

$M = D + O$ of order n

$$\Delta_m \equiv \det(D) \cdot \exp[\sum_{p=1}^{m} \frac{(-1)^p}{p} \operatorname{trace}((D^{-1}O)^p)]$$

If $\rho \equiv \rho(D^{-1}O) < 1$ then

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

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

If We Expand Long Enough ...

$M = D + O$ of order n

$$\Delta_m \equiv \det(D) \cdot \exp[\sum_{p=1}^{m} \frac{(-1)^p}{p} \operatorname{trace}((D^{-1}O)^p)]$$

If $c\rho^m < 1$ then

$$\left| \frac{\det(M) - \Delta_m}{\Delta_m} \right| \leq \frac{2n}{1-\rho} \rho^{m+1}$$

Zone Determinant Expansions

- New method for lattice simulation of finite temperature nuclear matter
- New expansion of nucleon matrix determinant in powers of boundary hopping parameter
- Simulations accelerated by factor $10^5 - 10^7$
- $1/\rho(D^{-1}O)$ $\simeq$ size of spatial zone
- $\mathrm{trace}((D^{-1}O)^p) = 0$ for p odd

Numerical Experiments

Realistic lattice simulation of interactions between neutrons and neutral pions

- $|\det(M)| \approx 10^6 \ldots 10^{29}$
- $\rho \equiv \rho(D^{-1}O) \approx .5$
- Once $c\rho^m < 1$ then

$$\left| \frac{\det(M) - \Delta_m}{\Delta_m} \right| \leq 4n\, \rho^{m+1}$$

Numerical Experiments

Complex non-Hermitian matrix

$$n = 3888, \quad \rho \approx .5122, \quad c\rho^m < 1 \text{ for } m \geq 12$$

$\ln(\det(M))$	$65.8009 - 0.7250\imath$
$\ln(\det(D))$	$51.3988 - 0.7888\imath$
$\ln(\Delta_2)$	$66.0028 - 0.7218\imath$
$\ln(\Delta_4)$	$65.8289 - 0.7243\imath$
$\ln(\Delta_6)$	$65.7926 - 0.7253\imath$
$\ln(\Delta_8)$	$65.8026 - 0.7249\imath$

Logarithm of Determinant

$M = D + O$ of order n

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

$$|\ln(\det(M)) - \ln(\Delta_m)| \leq \frac{n}{1-\rho} \rho^{m+1} \approx 5$$

Numerical experiments:

$$|\ln(\det(M)) - \ln(\Delta_m)| \approx 10^{-3}$$

Extension of Fischer & Hadamard

$$M = D + O$$

$$D = \begin{pmatrix} * & & \\ & * & \\ & & * \end{pmatrix} \qquad O = \begin{pmatrix} 0 & * & * \\ * & 0 & * \\ * & * & 0 \end{pmatrix}$$

If $\det(M)$ and $\det(D)$ real, D non-singular $\lambda_j(D^{-1}O) > -1$ real then

$$0 < \det(M) \le \det(D) \quad \text{or} \quad \det(D) \le \det(M) < 0$$

Summary

- $\det(M) = \exp(\mathrm{trace}(\log(M)))$
- Diagonal approximations $\det(M) \approx \det(D)$
- Sequence of higher order approximations
- Relative error bounds
- New method in quantum physics:
  Zone determinant expansion
- Extension of Fischer's and Hadamard's inequalities