Decay Properties of Certain Matrix Functions Arising in Quantum Mechanics

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In DFT, the electronic density ρ (a scalar field on $\mathbb{R}^3$) is sought, rather than the ground state wavefunction (a scalar field on $\mathbb{R}^{3N}$):

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For large systems, further approximations are necessary. In the LDA (Local Density Approximation) framework, the problem is reduced to the computation of a sequence of density matrices of certain one-electron Hamiltonians (SCF iteration).

Density Matrices

All the statistical properties of a quantum-mechanical system in a given state can be described by a density matrix, i.e., a compact (in fact, trace class) operator P on a Hilbert space $\mathcal{H}$ such that:

1. $0 \preceq P = P^*$
2. $\mathrm{Trace}(P) = 1$ ($\Rightarrow 0 \preceq P \preceq I$)
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For systems in equilibrium, $[H, P] = 0$ and P is a function of the Hamiltonian: $P = f(H)$.

Density Matrices

In practice, the operators are replaced by matrices upon introduction of a set of basis functions $\{\phi\}_{i=1}^{n}$ into the Hilbert space $\mathcal{H}$, where n is a multiple of $N = \#$ of electrons. For simplicity, here we assume an orthonormal basis. The resulting matrices are 'sparse': their pattern/bandwidth is determined by the *range* of the interactions.

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4. The uncertainty (dispersion) of an observable:
   $\Delta A = (\langle A^2 \rangle - \langle A \rangle^2)^{\frac{1}{2}} = [\text{Trace}(A^2 P) - \text{Trace}(AP)^2]^{\frac{1}{2}}$

Density Matrices

In (zero-temperature) electronic structure theory P is, up to a normalization factor, the spectral projector onto the subspace spanned by the N lowest eigenfunctions of H (occupied states):

$$P = \frac{1}{N}\left(\psi_1\psi_1^* + \cdots + \psi_N\psi_N^*\right)$$

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Ignoring the normalization factor, $P = f(H)$ where f is the step function

$$f(x) = \begin{cases} 1 & \text{if} \quad x \le \mu \\ 0 & \text{if} \quad x > \mu \end{cases}$$

with $\lambda_N \le \mu < \lambda_{N+1}$ ("Fermi level").

Density Matrices

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This expression for P is obtained by maximizing the 'von Neumann entropy' $\sigma = -\text{Trace}(P \log P)$ subject to $\text{Trace}(P) = 1$ and $\text{Trace}(HP) = \langle H \rangle$.

Approximations of P

$$f(x) = \frac{1}{1 + e^{\beta(x-\mu)}}$$

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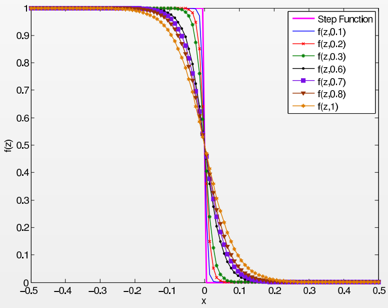

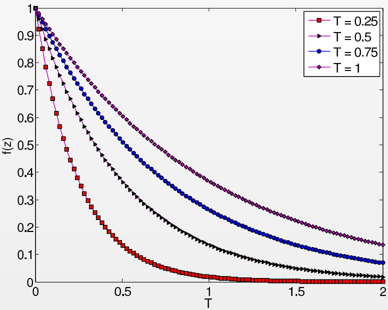

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- In the last 10-15 years, this localization property has been exploited to develop 'linear scaling' algorithms for approximating P, i.e., algorithms that asymptotically require $O(n) = O(kN)$ work
- There are also connections with random matrix theory and with the deflation phenomenon in the Divide-and-Conquer algorithm for the eigenvalues of symmetric tridiagonal matrices; see Trefethen and Bau's *Numerical Linear Algebra*, pp. 232–233 ▸ More

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Since we are interested in $\text{Trace}(PA)$ for different A, we need to compute P (to a certain accuracy). Diagonalization costs $O(n^3)$ work and $O(n^2)$ storage $\Rightarrow$ too expensive!

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- Answer
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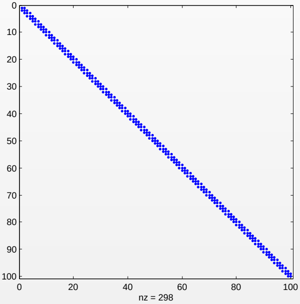
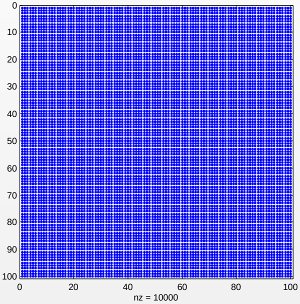
- An important goal:
  To investigate the possibility of linear scaling algorithms to approximate $f(A)$ when A is sparse (or banded), and to develop such $O(n)$ methods when appropriate

An example for e^A with A tridiagonal

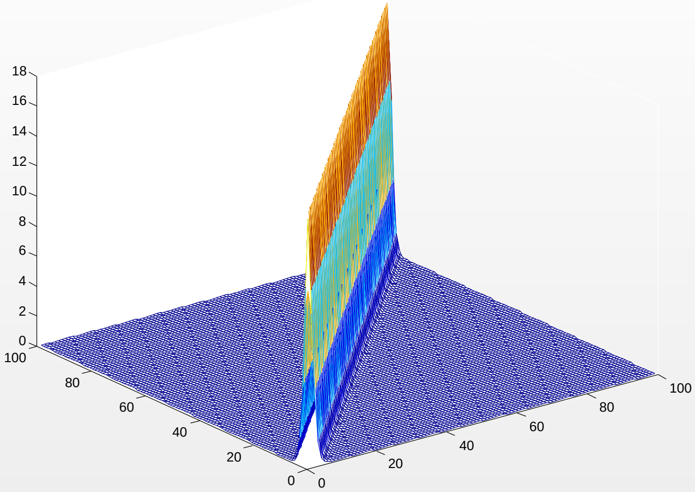
Sparsity pattern of $A = \text{trid}(-1, 2, -1)$ and $e^A = \texttt{expm}(A)$.





An example for e^A with tridiagonal A

$|[e^A]_{ij}|$



A decay result for functions of banded symmetric matrices

Theorem

Let A be a symmetric m-banded matrix and let f be a smooth function on the spectrum of A such that $f(x)$ is real for $x \in \mathbb{R}$. Then there exist $0 < \rho < 1$ and $K = K(f, A)$ such that $|[f(A)]_{ij}| \leq K\rho^{|i-j|}$.

Main ingredients of the proof: approximation theory (Bernstein's Thm.) and the Spectral Theorem.

Also valid for $A \in \mathcal{B}(\ell^2)$ if $f(A) \in \mathcal{B}(\ell^2)$.

M. B. & Gene Golub, Bounds for the entries of matrix functions with applications to preconditioning, BIT, 1999

Brief review of decay results

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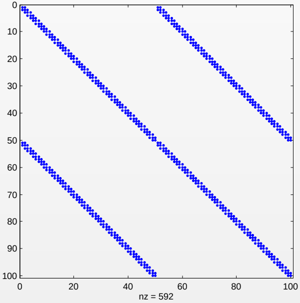
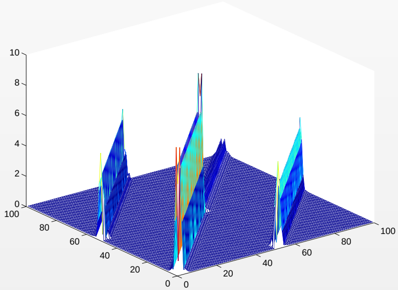
- In 2006, extensions of the B.-Golub bounds to sparse Hermitian matrices appeared in the quantum computing literature
- Further extension to non-normal matrices by B. & Razouk in 2007

Decay for exponential of a sparse Hamiltonian matrix

Sparsity pattern of a $2n \times 2n$ Hamiltonian matrix A and decay in $\exp(A)$.

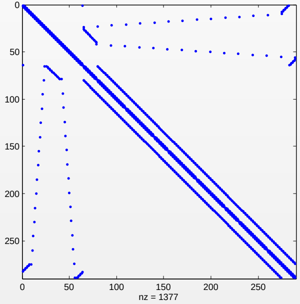


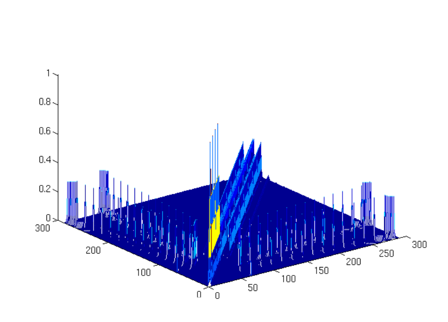


Note that $\exp(A)$ is symplectic. Also, here A is non-normal.

Decay for logarithm of a sparse matrix

Sparsity pattern of $A =$ `mesh3e1` (from NASA) and decay in $\log(A)$.

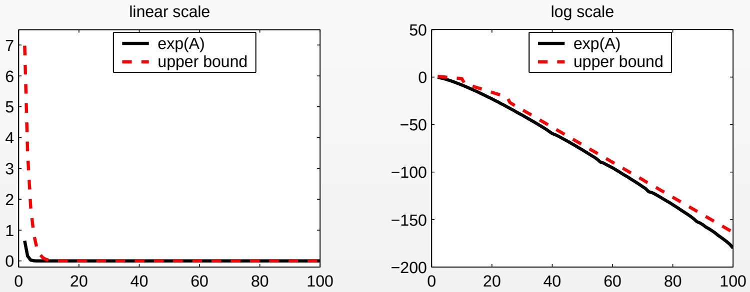




Here A is symmetric positive definite.

Assessment of the bound for A banded Hermitian

Upper bounds vs. $|[e^A]_{ij}|$ first row.



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Sufficient conditions for $O(n)$ approximation of $f(A)$

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- The result holds for any sparsity pattern of $\{A_n\}$ (independent of n)

Approximation of $f(A)$ by polynomials

Algorithm ▸ More

- We compute approximations of $f(A)$ using Chebyshev polynomials
  - The degree of the polynomial can be estimated a priori
  - The coefficients of the polynomial can be pre-computed (indep. of n)
  - Estimates for the extreme eigenvalues of A are required
- The polynomial expansion is combined with a procedure that a priori determines a bandwidth or sparsity pattern for $f(A)$ outside which the elements are so small that they can be neglected

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Cost

This method is multiplication-rich; the matrices are kept sparse throughout the computation, hence $O(n)$ arithmetic and storage requirements. Matrix polynomials are evaluated with the classical Paterson-Stockmeyer algorithm.

Decay bounds for the Fermi-Dirac approximation

Assume that H is m-banded and has spectrum in $[-1, 1]$, then

$$\left| \left[\left(I + e^{\beta(H-\mu I)} \right)^{-1} \right]_{ij} \right| \le K(\gamma)\rho(\gamma)^{\frac{2|i-j|}{m}}.$$

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We choose β and $\hat{m}$ so as to guarantee an accuracy $\|P - f(H)\|_2 < 10^{-6}$.

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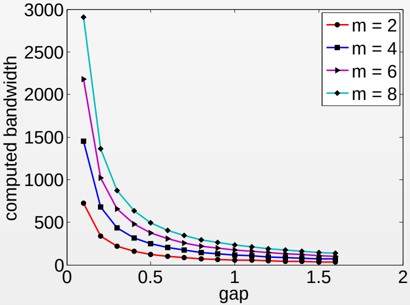
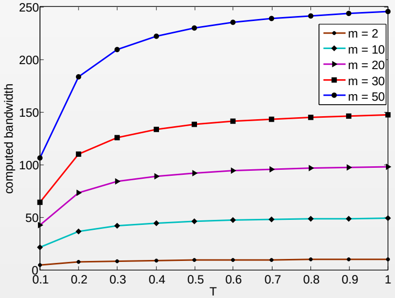
Remark: The above bound only depends on m and γ.

Computed bandwidth for approximations of P

$$f(x) = \frac{1}{1 + e^{\beta(x-\mu)}} \qquad\qquad f(x) = e^{-\frac{x}{\kappa T}}$$





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Our bounds, depending only on the interaction range m and on the spectral gap γ, are *a priori* and provide a justification of linear scaling algorithms. However, some estimate of γ is needed.

Overview

Chebyshev expansion

Some results for A_n tridiagonal, SPD

	$A \log(A)$	$\text{Trace}[A \log(A)]$		
n	rel. error	error	$\hat{m}$	k
100	$5e{-}07$	$3e{-}04$	20	9
200	$6e{-}07$	$8e{-}04$	20	9
300	$1e{-}07$	$3e{-}04$	20	10
500	$2e{-}07$	$5e{-}04$	20	10

In the Table, $\hat{m}$ is the estimated bandwidth and k is the number of terms in the Chebyshev expansion. Note the $O(n)$ behavior in terms of cost.

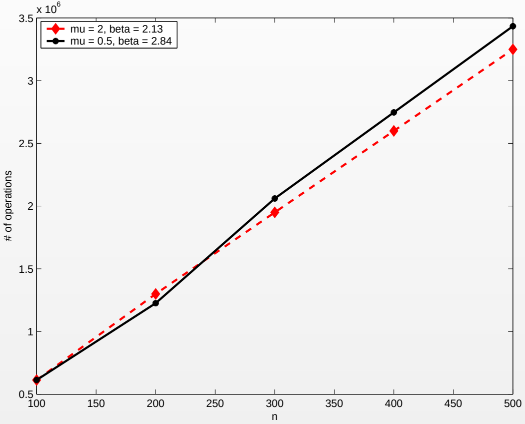
Density matrix computation (toy example)

The bandwidth was computed prior to the calculation to be ≈ 20; here H is tridiagonal (1D Anderson model).

Table: Results for $f(x) = \frac{1}{1+\mathrm{e}^{(\beta(x-\mu))}}$

	$\mu = 2,\ \beta = 2.13$			$\mu = 0.5,\ \beta = 1.84$		
n	error	k	$\hat{m}$	error	k	$\hat{m}$
100	$9e{-}06$	18	20	$6e{-}06$	18	22
200	$4e{-}06$	19	20	$9e{-}06$	18	22
300	$4e{-}06$	19	20	$5e{-}06$	20	22
400	$6e{-}06$	19	20	$8e{-}06$	20	22
500	$8e{-}06$	19	20	$8e{-}06$	20	22

Density matrix computation



The $O(n)$ behavior of Chebyshev's approximation to the Fermi–Dirac function $f(H) = (\exp(\beta(H - \mu I)) + I)^{-1}$.

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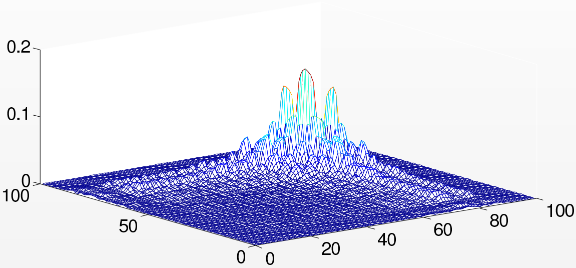
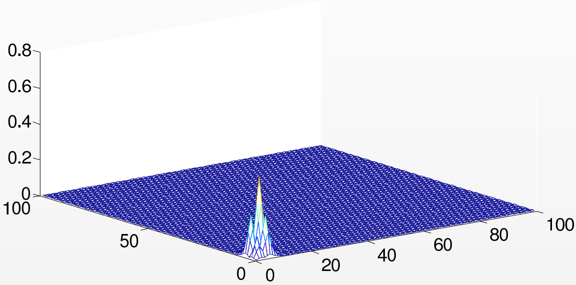
An excellent reference: C. LeBris, *Computational Chemistry from the Perspective of Numerical Analysis*, Acta Numerica 14 (2005), 363-444.

Localization in spectral projectors: small gap



Rank-one spectral projector for $A = A^T$ tridiagonal. Relative gap $\gamma = 10^{-3}$. Note the slow decay and oscillatory behavior.

Localization in spectral projectors: large gap



Rank-one spectral projector for $A = A^T$ tridiagonal. Relative gap $\gamma = 0.5$.

Back

Chebyshev approximation

For A with $\sigma(A) \subset [-1, 1]$ the Chebyshev polynomials are given by

$$T_{k+1}(A) = 2AT_k(A) - T_{k-1}(A),\ T_1(A) = A,\ T_0(A) = I.$$

Then $f(A)$ can be represented in a series of the form

$$f(A) = \sum_{k=0}^{\infty} c_k T_k(A).$$

The coefficients of the expansion are given by

$$c_k \approx \frac{2}{M} \sum_{j=1}^{M} f(\cos(\theta_j)) \cos((k-1)\theta_j),$$

where $\theta_j = \pi(j - \frac{1}{2})/M$. Back

The n-independence of the error

The Nth truncation error without dropping can be written as

$$\|e_N(A)\| = \|f(A) - \sum_{k=0}^{N} c_k T_k(A)\|.$$

For x in $[-1,1]$ we have that $|T_k(x)| \leq 1$ for $k = 1, 2, \ldots$. Then

$$\|e_N(A)\| = \| \sum_{k=N+1}^{\infty} c_k T_k(A)\| \leq \sum_{k=N+1}^{\infty} |c_k|.$$

Back

A Theorem of Bernstein

The set of Faber polynomials can be used to obtain a uniform approximation to an analytic function f with a sequence of polynomials of bounded degree, i.e.,

$$|f(z) - \Pi_N(z)| < cq^N \quad (0 < q < 1)$$

for all $z \in F$, where c and q depend on the analytic properties of f.

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Example – Disk

If the region is a disk of radius ρ centered at z_0, then for any function f analytic on the disk of radius ρ/q centered at z_0, where $0 < q < 1$, there exists a polynomial Π_N of degree at most N and a positive constant c such that

$$|f(z) - \Pi_N(z)| < cq^N,$$

for all $z \in F$.

Back