Exponentially Localised Matrices

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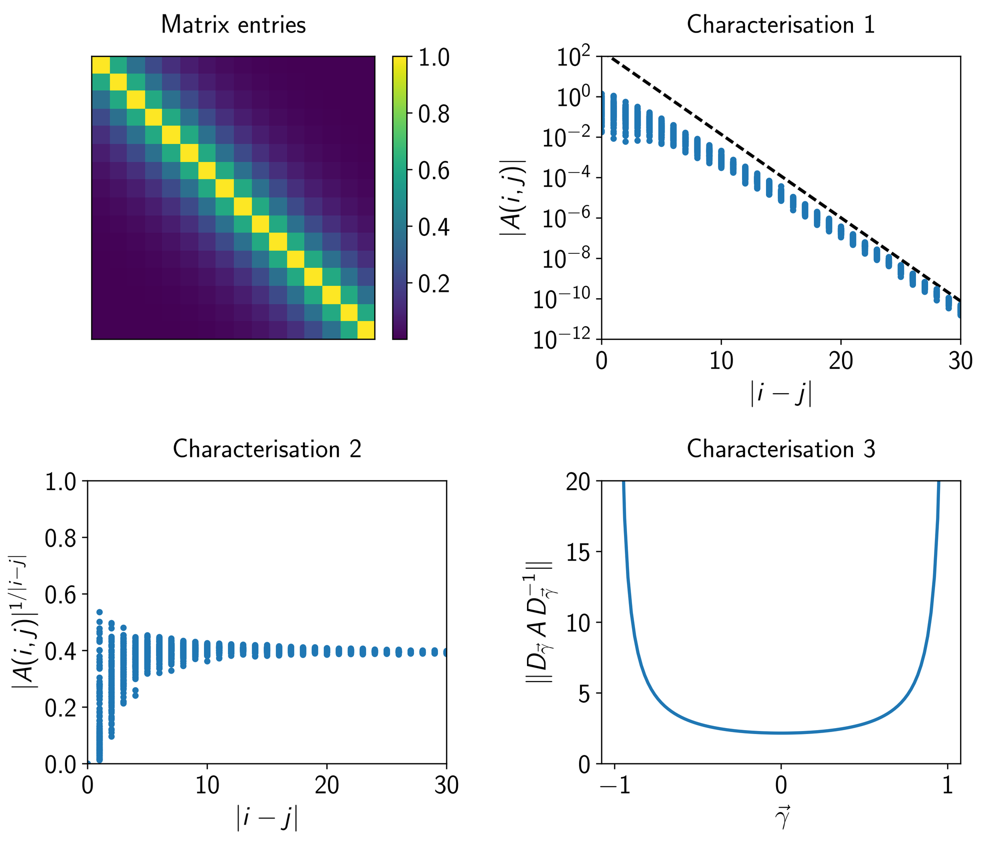
Exponential Localisation

Definition. *An infinite matrix $A \in \mathcal{L}(\ell_2(\mathbb{Z}^d))$ is called* exponentially localised with rate $\gamma > 0$ *if it satisfies the following three equivalent properties:*

1. *For each $\tilde\gamma \in [0, \gamma)$ there exists a $C > 0$ such that*
$$|A(i,j)| \le C \exp(-\tilde\gamma\,|i-j|) \qquad \forall i,j \in \mathbb{Z}^d.$$
2. *For each diverging sequence $s_n \in \mathbb{Z}^d$ we have, uniformly for all $i \in \mathbb{Z}^d$,*
$$\limsup_{n\to\infty} |A(i, i+s_n)|^{1/|s_n|} \le \exp(-\gamma).$$
3. *For each $\vec\gamma \in \mathbb{R}^d$, $|\vec\gamma| < \gamma$, and $p \in [0,\infty]$, it holds $\|D_{\vec\gamma} A D_{\vec\gamma}^{-1}\|_p$ is finite, where $D_{\vec\gamma} \in \mathcal{L}(\ell_2(\mathbb{R}^d))$ is defined through $(D_{\vec\gamma}\,x)(i) = \exp(\vec\gamma\cdot i)\,x(i)$.*

The set of all such matrices is denoted by $Loc(\gamma)$.

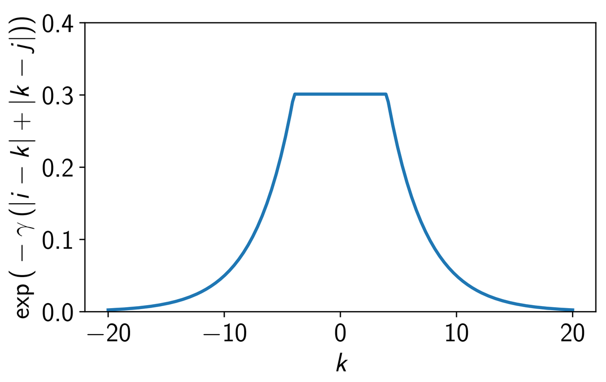


Product of Exponentially Localised Matrices

Theorem.
$$A \in Loc(\gamma_A),\ B \in Loc(\gamma_B) \implies AB \in Loc(\min\{\gamma_A, \gamma_B\}).$$

Proof. For any $\vec\gamma_{AB} \in \mathbb{R}^d$ with $|\vec\gamma_{AB}| < \min\{\gamma_A,\gamma_B\}$, we have
$$\|D_{\vec\gamma_{AB}} AB D_{\vec\gamma_{AB}}^{-1}\|_p \le \|D_{\vec\gamma_{AB}} A D_{\vec\gamma_{AB}}^{-1}\|_p\,\|D_{\vec\gamma_{AB}} B D_{\vec\gamma_{AB}}^{-1}\|_p \le C.$$
□

This theorem would not hold if we had defined exponential localisation as
$$Loc'(\gamma) := \{A \in \mathcal{L}(\ell_2(\mathbb{Z}^d)) \mid \exists C > 0 : |A(i,j)| \le C\,\exp(-\gamma\,|i-j|)\}.$$
This is easy to see in one dimension. Assume $A, B \in Loc'(\gamma)$ and $i < j$. Then,
$$\begin{aligned} |(AB)(i,j)| &\le C \sum_{k=-\infty}^{\infty} \exp\big(-\gamma\,(|i-k| + |k-j|)\big) \\ &= C\left(\sum_{k=i}^{j} \exp\big(-\gamma\,(j-i)\big) + \sum_{\substack{k=-\infty,\dots,i-1,\\ j+1,\dots,\infty}} \exp\big(-\gamma\,|2k-i-j|\big)\right) \\ &= C\left(1 + |i-j| + \frac{2}{\exp(2\gamma)-1}\right) \exp\big(-\gamma\,|i-j|\big). \end{aligned}$$



Applications

Linear Scaling Algorithms
The above definition of exponential localisation for infinite matrices $A \in \mathcal{L}(\ell_2(\mathbb{Z}^d))$ can be adapted to sequences of finite-size matrices $A_n \in \mathbb{C}^{n\times n}$ by requiring that the parameters and bounds in the definition are independent of n. If a matrix $A \in \mathbb{C}^{n\times n}$ is localised in this sense, we can approximate it by a banded matrix and thereby reduce both the storage complexity as well as the computational costs for matrix products and factorisations to $\mathcal{O}(n)$.

Localisation of Perturbations
Exponential localisation of $A \in Loc(\gamma)$ implies that a perturbation of a vector $x \in \ell_2(\mathbb{Z}^d)$ at a position $i \in \mathbb{Z}^d$ only has an exponentially small impact on the entries of Ax far away from i. This is useful in numerical analysis, as it implies for example convergence of domain truncation methods.

Functions of Exponentially Localised Matrices

Theorem. *Let $A \in Loc(\gamma)$, and let $f : \sigma(A) \to \mathbb{C}$ be analytic. Then, $f(A) \in Loc(\hat\gamma)$ for some $\hat\gamma > 0$.*

Common examples for $f(z)$ are
$$f(z) = z^{-1} \qquad\text{or}\qquad f(z) = \begin{cases} 1 & \text{if } z \in X, \\ 0 & \text{otherwise,}\end{cases}$$
where $X \subset \mathbb{C}$ such that $\partial X \cap \sigma(A) = \{\}$. The latter choice allows to estimate the localisation of eigenvectors corresponding to isolated eigenvalues.

Neumann Approach [CT73]

The case of general function $f(z)$ can be reduced to the particular case of $f(z) = z^{-1}$ using the Cauchy contour integral formula
$$f(A) = \frac{1}{2\pi\iota}\oint_{\partial\Omega} f(z)\,(z-A)^{-1}\,dz$$
where $\Omega \subset \mathbb{C}$ is an open set such that $\sigma(A) \subset \Omega$ and f can be analytically extended to Ω.

We thus aim to find $\hat\gamma > 0$ such that $\|D_{\vec\gamma}\,A^{-1}\,D_{\vec\gamma}^{-1}\|_p < \infty$ for all $\vec\gamma \in \mathbb{R}^d$ with $|\vec\gamma| < \hat\gamma$. To this end, we will use the following result.

Lemma (Neumann). *Let A, B be two operators such that A is boundedly invertible and $\|B - A\| < \|A^{-1}\|^{-1}$. Then, B is boundedly invertible.*

This lemma guarantees $\|D_{\vec\gamma}\,A^{-1}\,D_{\vec\gamma}^{-1}\|_p < \infty$ for all $\vec\gamma \in \mathbb{R}^d$, $|\vec\gamma| < \hat\gamma$, if
$$a_p(\hat\gamma) := \sup_{|\vec\gamma| = \hat\gamma} \|A - D_{\vec\gamma}\,A\,D_{\vec\gamma}^{-1}\|_p < \|A^{-1}\|_p^{-1}.$$
Assuming $a : \mathbb{R}_{\ge 0} \to \mathbb{R}_{\ge 0}$ is bijective, this yields $\hat\gamma = a_p^{-1}(\|A^{-1}\|_p^{-1})$.

We can easily estimate $a_p(\hat\gamma)$ for important classes of matrices:

Laplacian-like:
$$A(i,j) = \begin{cases} a_i \in \mathbb{C} & \text{for } |i-j| = 0 \\ -1 & \text{for } |i-j| = 1 \\ 0 & \text{for } |i-j| > 1 \end{cases} \implies a_p(\hat\gamma) \le 2d\,\sinh(\hat\gamma).$$

Exponential localisation:
$$|A(i,j)| \le C\exp(-\gamma\,|i-j|) \implies a_p(\hat\gamma) \le \frac{Cd\,\sinh(\hat\gamma)}{\cosh(\gamma) - \cosh(\hat\gamma)}.$$

Gaussian localisation:
$$|A(i,j)| \le C\exp(-\gamma\,|i-j|^2) \implies a_p(\hat\gamma) \le Cd\,\sqrt{\tfrac{\pi}{\gamma}}\,\operatorname{erf}\!\left(\tfrac{\hat\gamma}{2\sqrt{\gamma}}\right)\exp\!\left(\tfrac{\hat\gamma^2}{4\gamma}\right).$$

Polynomial Approximation Approach

This approach only applies to a subset of exponentially localised matrices.

Definition (banded matrix). *A matrix $A \in \mathcal{L}(\ell_2(\mathbb{Z}^d))$ is called m-banded if*
$$|i-j| > m \quad\implies\quad A(i,j) = 0 \qquad \forall i,j \in \mathbb{Z}^d.$$
The set of all such matrices is denoted by $Band(m)$.

Theorem ([DMS84]). *Let $A \in Band(m)$ and $f : \sigma(A) \to \mathbb{C}$. Then,*
$$|f(A)(i,j)| \le \inf_{p_k \in \mathcal{P}_k} \|f - p_k\|_{\infty,\sigma(A)} \qquad \forall i,j \in \mathbb{Z}^d,\ k = \left\lfloor \tfrac{|i-j|-1}{m} \right\rfloor.$$

Proof. Let $p_k \in \mathcal{P}_k$, which by the choice of k implies $p_k(A)(i,j) = 0$. Hence
$$\begin{aligned} |f(A)(i,j)| &\le |p_k(A)(i,j)| + |f(A)(i,j) - p_k(A)(i,j)| \\ &\le 0 + \|f(A) - p_k(A)\|_2 \\ &\le \|f - p_k\|_{\infty,\sigma(A)}. \end{aligned}$$
□

The localisation of $f(A)$ with $A \in Band(m)$ is thus determined by how well f can be approximated using polynomials. We have the following result from logarithmic potential theory.

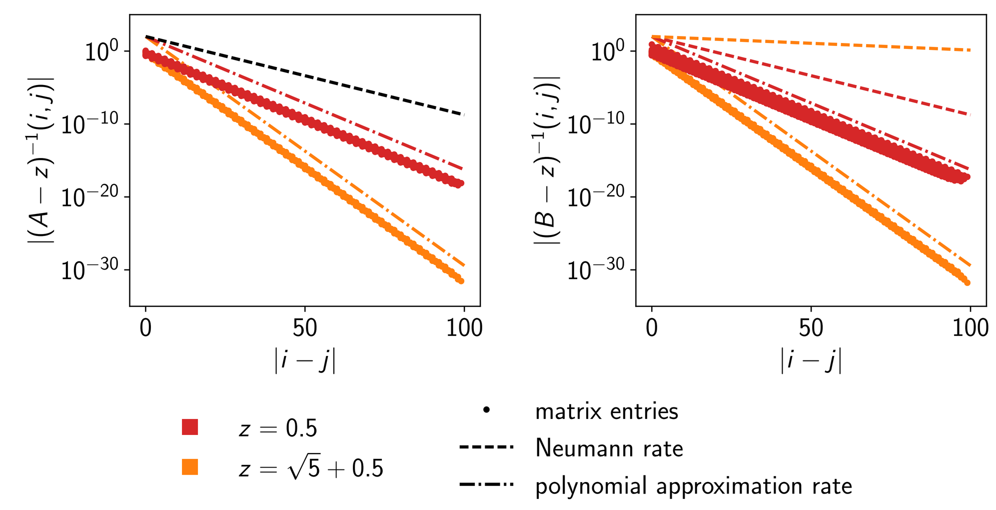
Theorem. *Let $\sigma \subset \mathbb{C}$ be compact such that σ^c is connected, and let $f : \sigma \to \mathbb{C}$ be analytic. There exists a function $g : \mathbb{C} \to [0,\infty)$ depending only on $\overline{\sigma^\circ}$, called the* Green's function of σ^c*, such that*
$$\lim_{k\to\infty}\inf_{p_k \in \mathcal{P}_k} \|f - p_k\|_{\infty,\sigma}^{1/k} = \exp(-g^\star)$$
where
$$g^\star := \max\left\{\tilde g > 0 \mid f \text{ can be analytically extended to } \{z \in \mathbb{C} | g(z) < \tilde g\}\right\}.$$

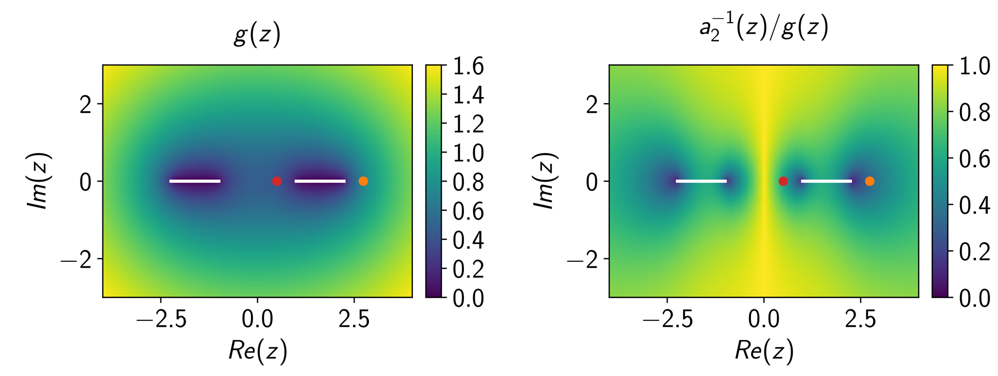
Proof. See e.g. [Ran95]. □

Physically, $g(z)$ corresponds to the electrostatic potential of a metal σ carrying a unit charge. Examples for (σ, g) pairs are
$$\sigma = [-1,1] \implies g(z) = \log\left(\left|z + \sqrt{z^2-1}\right|\right),$$
$$\sigma = [a,b]\cup[c,d] \implies g(z) = \operatorname{Re}\left(\int_a^z \frac{(s-u)\,du}{\sqrt{(u-a)\,(u-b)\,(u-c)\,(u-d)}}\right).$$
In the second case, $a < b < c < d \in \mathbb{R}$ and
$$s = \frac{\int_b^c \frac{u\,du}{\sqrt{(u-a)\,(u-b)\,(u-c)\,(u-d)}}}{\int_b^c \frac{du}{\sqrt{(u-a)\,(u-b)\,(u-c)\,(u-d)}}}.$$
The Green's function for two intervals was derived in [SSW01].

Numerical Experiments

Laplacian-like Matrix
Let us consider the two matrices $A, B \in \mathbb{C}^{100\times 100}$ with entries
$$A(i,j) := \begin{cases} (-1)^i & \text{if } |i-j| = 0, \\ -1 & \text{if } |i-j| = 1, \\ 0 & \text{if } |i-j| > 1, \end{cases} \qquad B(i,j) := \begin{cases} 0 & \text{if } i = j = 1, \\ A(i,j) & \text{otherwise.}\end{cases}$$
and spectra
$$\sigma(A) \subset [-\sqrt5, -1] \cup [1, \sqrt5], \qquad \sigma(B) \subset \sigma(A) \cup \{0.4142\}.$$

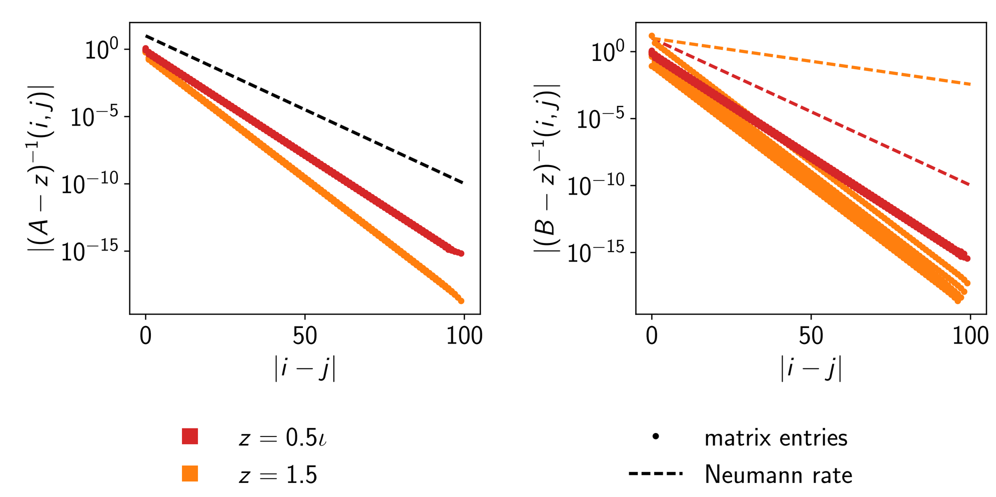




We observe:

- The localisation rate depends on all of $\sigma(A - z)$, not just $\min|\sigma(A-z)|$.
- Isolated points do not affect the localisation rate.
- The polynomial approximation approach yields the exact localisation rate. In particular, it correctly predicts the previous two points.
- The Neumann bound is reasonably sharp for large $\|A^{-1}\|_2^{-1}$ but deteriorates arbitrarily for $\|A^{-1}\|_2^{-1} \to 0$.

Exponentially Localised Matrix
We next consider the matrices $A, B \in \mathbb{C}^{100\times 100}$ with entries
$$A(i,j) := m\exp(-|i-j|) + b\,\delta_{ij}, \qquad B(i,j) := \begin{cases} 1.4 & \text{if } i = j = 1, \\ A(i,j) & \text{otherwise,}\end{cases}$$
where $m, b \in \mathbb{R}$ are chosen such that
$$\sigma(A) \subset [-1,1],\ -1, 1 \in \sigma(A), \qquad \sigma(B) \subset \sigma(A) \cup \{1.5577\}.$$



Discussion

The Neumann approach for proving localisation of the inverse applies to any matrix $A \in Loc(\gamma)$ and mostly estimates the localisation rate with reasonable accuracy. It gives very wrong results, however, if there is an isolated eigenvalue close to the origin. It would be useful if the Neumann approach could be adapted to reflect this fact, or if the polynomial approximation approach could be extended to arbitrary localised matrices.

References

[CT73] J. M. Combes and L. Thomas, *Asymptotic Behaviour of Eigenfunctions for Multiparticle Schrödinger Operators*, Communications in Mathematical Physics, 34 (1973), pp. 251–270, doi:10.1007/BF01646473.

[DMS84] S. Demko, W. F. Moss, and P. W. Smith, *Decay Rates for Inverses of Band Matrices*, Mathematics of Computation, 43 (1984), pp. 491–499, doi:10.1090/S0025-5718-1984-0758197-9.

[Ran95] T. Ransford, *Potential Theory in the Complex Plane*, Cambrige University Press, 1995.

[SSW01] J. Shen, G. Strang, and A. J. Wathen, *The Potential Theory of Several Intervals and Its Applications*, Applied Mathematics and Optimization, 44 (2001), pp. 67–85, doi:10.1007/s00245-001-0011-0.