Linear-Scaling Approximate Factorisation and Selected Inversion for Electronic Structure Models

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IWR School, 2 - 6 October 2017

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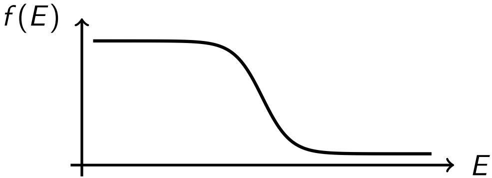
Introduction

Task

Given symmetric Hamiltonian $H \in \mathbb{R}^{n \times n}$, compute total energy

$$E_{tot} := \operatorname{Tr}\big(H\, f(H)\big), \qquad f(E) := \frac{1}{1 + \exp\big(\beta\,(E - \mu)\big)}.$$



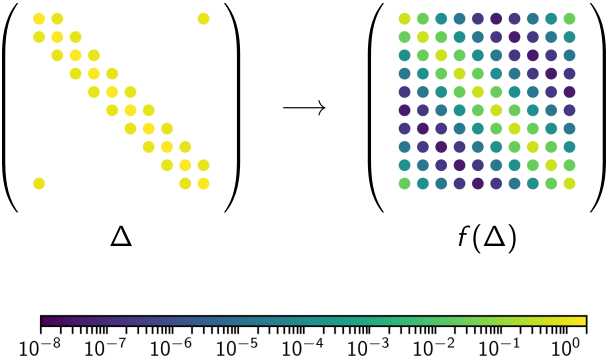
Introduction

Diagonalisation

Compute eigenvalues E_k of H and evaluate

$$E_{tot} := \sum_{k=1}^{n} E_k \, f(E_k).$$

Localisation



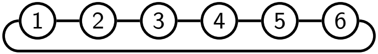
Matrx Graphs

Graph of Sparse Matrix $A \in \mathbb{R}^{n \times n}$
Graph $G(A) := \big(V(A), E(A)\big)$ defined by

$$V(A) := \{1, \ldots, n\}, \qquad E(A) := \{(i,j) \mid A(i,j) \neq 0\}.$$

Example

$$\begin{pmatrix} 1 & \bullet & & & & \bullet \\ \bullet & 2 & \bullet & & & \\ & \bullet & 3 & \bullet & & \\ & & \bullet & 4 & \bullet & \\ & & & \bullet & 5 & \bullet \\ \bullet & & & & \bullet & 6 \end{pmatrix}$$



Localisation

Theorem [DMS84]

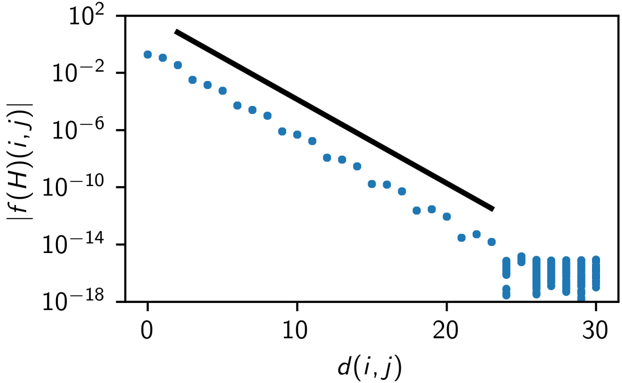
$$|f(H)(i,j)| \leq \inf_{p \in \mathcal{P}_{d(i,j)-1}} \|f - p\|_{\infty,\sigma(H)}$$

Proof.

$$\begin{aligned} |f(H)(i,j)| &\leq |p(H)(i,j)| + |f(H)(i,j) - p(H)(i,j)| \\ &\leq \|f - p\|_{\infty,\sigma(H)}. \end{aligned}$$

[DMS84] S. Demko, W. F. Moss and P. W. Smith. *Decay Rates for Inverses of Band Matrices. Mathematics of Computation* (1984)

Localisation



PEXSI Algorithm

Pole Expansion and Selected Inversion (PEXSI) [Lin+13]

- Rewrite total energy using contour integral:

$$E_{tot} = \mathrm{Tr}\left(H\,f(H)\right) = \frac{1}{2\pi\iota}\int_{\gamma} z\,f(z)\ \mathrm{Tr}\left(\left(z-H\right)^{-1}\right)dz.$$

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- For each quadrature point z, do
  - Compute factorisation $LDL^T := z - H$.
  - Compute $(z - H)^{-1}(i, j)$ for few i, j using L and D.

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Sparse Factorisation

Fill Path

Path $i, k_1, \ldots, k_p, j$ in $G(A)$ such that $k_1, \ldots, k_p < \min\{i, j\}$.

[RT78] D. J. Rose and R. E. Tarjan. *Algorithmic Aspects of Vertex Elimination on Directed Graphs. SIAM Journal on Applied Mathematics* (1978)

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Fill Path Theorem [RT78]
Let $A = LDL^T$. Barring cancellation, it holds

$$(L + L^T)(i,j) \neq 0 \iff i, j \text{ are connected by a fill path.}$$

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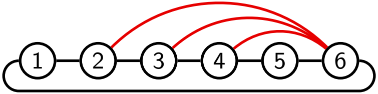

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Localisation of Factorisation

Level-of-fill

$$level(i, j) := \min\{length(P) - 1 \mid P \text{ is a fill path connecting } i \text{ and } j\}.$$

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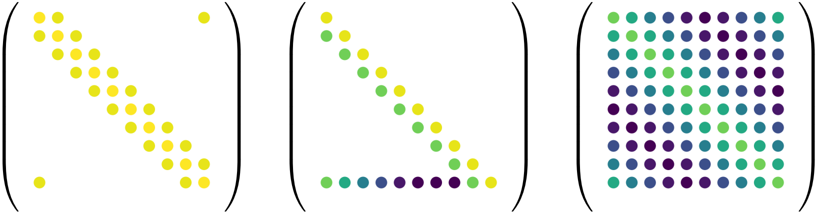
Theorem

Let $LDL^T := H$. Then,

$$|L(i,j)| \leq \inf_{p \in \mathcal{P}_{level(i,j)-1}} \|f - p\|_{\infty, \sigma(A(\{1,\ldots,j-1\},\{1,\ldots,j-1\}))}.$$



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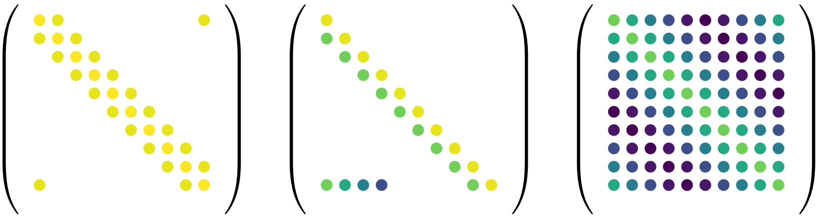

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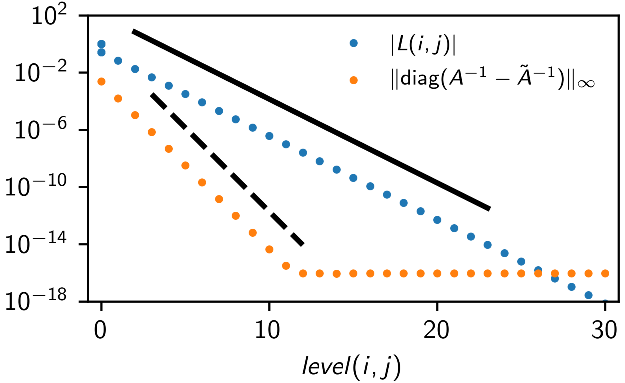
Incomplete Sparse Factorisation



Cramer's Rule

Cramer's rule

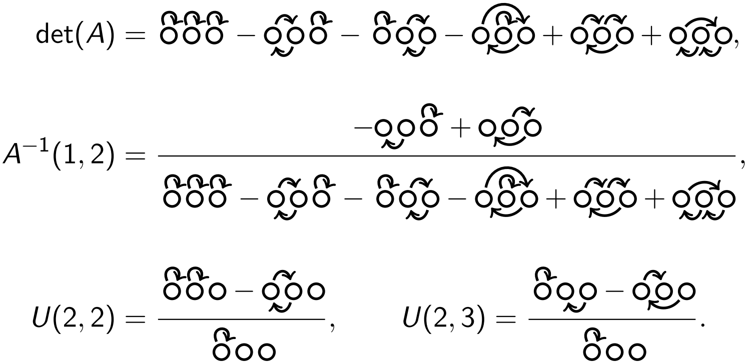
$$A^{-1}(i,j) = (-1)^{i+j}\,\frac{\det\left(A^c_{ji}\right)}{\det(A)}.$$

Determinant

$$\det(A) := \sum_{p \in P_n} \operatorname{sgn}(p) \prod_{i=1}^{n} A(p_i, i).$$

Cramer's Rule

Illustration with $A = LU \in \mathbb{R}^{3\times 3}$



LU factorisation closely related to Floyd-Warshall algorithm.

Cramer's Rule

Conjecture
Error in incomplete factorisation results because certain improper paths no longer cancel.

Conjecture
Long paths contribute exponentially little to Cramer's rule.

Conclusion

Incomplete Sparse Factorisation and Selected Inversion
Linear-scaling algorithm with reduced-order scaling even without localisation.

Cramer's rule

- Could be helpful to analyse incomplete factorisation.
- Potentially new approach to localisation.

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