Tensor trains for high-dimensional problems

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Contents

Introduction

These notes are a short introduction to the tensor train decomposition, with a particular focus on solving linear equations within this format. The tensor train decomposition [OT09] is presented as a generalisation of the singular value decomposition for matrices, which is central in the characterisation of the low-rank approximation problem. Approximation results for the tensor train format as well as the tensor train manifold are discussed.

The second part deals with the numerical resolution of linear systems or eigenvalue problems. The historical algorithm is an alternating scheme, known as the density matrix renormalisation group (DMRG) [Whi92, HRS12a], using the variational formulation of symmetric linear problems. Another way to solve linear problems is to adapt the classical iterative methods to the tensor train format [KU16]. Both approaches are presented and discussed in the present notes.

These notes are inspired by the following texts on the tensor train decomposition [Hac12, Hac14, Sch11, BSU16, UV20, Bac23].

Chapter 1

Tensor trains

1.1 Singular value decomposition and generalisations for tensors

This chapter is devoted to the tensor train decomposition, as a generalisation of the singular value decomposition (SVD) for high-dimensional tensors. The SVD arises in the low-rank approximation of matrices, as such, it is natural to look for generalisation of the SVD for high-dimensional tensors. As it will be mentioned, the historical tensor formats, i.e. the CP decomposition and the Tucker decomposition suffer from drawbacks that the tensor train format does not have.

1.1.1 The low-rank approximation for matrices

The basis tool for the low-rank approximation of matrices is the singular value decomposition (SVD).

Theorem 1.1.1 (Singular value decomposition)**.** *Let $A \in \mathbb{R}^{m\times n}$ be a matrix. There exist orthogonal matrices $U \in \mathbb{R}^{m\times r_A}$ and $V \in \mathbb{R}^{n\times r_A}$, and a diagonal matrix $\Sigma = \mathrm{Diag}(s_1, \ldots, s_{r_A})$ with $s_1 \geq \cdots \geq s_{r_A} > 0$ such that $A = U\Sigma V^{\mathsf{T}}$. The triplet of matrices $(U, \Sigma, V^{\mathsf{T}})$ satisfying these properties is called a singular value decomposition (SVD) of A.*

The SVD given in the above theorem is sometimes called the *compact* SVD of A. Another common definition of the SVD is a decomposition of the matrix $A \in \mathbb{R}^{m\times n}$ is to write the SVD as $A = \mathcal{U}\boldsymbol{\Sigma}\mathcal{V}^{\mathsf{T}}$ where $\mathcal{U} \in \mathbb{R}^{m\times m}$ and $\mathcal{V} \in \mathbb{R}^{n\times n}$ are orthogonal matrices and $\boldsymbol{\Sigma} \in \mathbb{R}^{m\times n}$ is diagonal. The relationship between this SVD and its compact version is the following

$$\mathcal{U} = \begin{bmatrix} U & 0 \end{bmatrix}, \quad \boldsymbol{\Sigma} = \begin{bmatrix} \Sigma & 0 \\ 0 & 0 \end{bmatrix}, \quad \mathcal{V} = \begin{bmatrix} V & 0 \end{bmatrix}.$$

The SVD of A can be derived from the eigenvalue decomposition of the matrices AA^T and AA^T. Indeed, if $A = \mathcal{U}\Sigma\mathcal{V}^\mathsf{T}$ is the SVD of A, then $A^\mathsf{T} = \mathcal{V}\Sigma\mathcal{U}^\mathsf{T}$ so using that $\mathcal{U}$ and $\mathcal{V}$ are orthogonal matrices, we have

$$AA^\mathsf{T} = \mathcal{U}\Sigma\Sigma^\mathsf{T}\mathcal{U}^\mathsf{T} = \mathcal{U}\begin{bmatrix} s_1^2 & & & & \\ & \ddots & & & \\ & & s_r^2 & & \\ & & & 0 & \\ & & & & \ddots \end{bmatrix}\mathcal{U}^\mathsf{T}, \quad A^\mathsf{T}A = \mathcal{V}\Sigma^\mathsf{T}\Sigma\mathcal{V}^\mathsf{T} = \mathcal{V}\begin{bmatrix} s_1^2 & & & & \\ & \ddots & & & \\ & & s_r^2 & & \\ & & & 0 & \\ & & & & \ddots \end{bmatrix}\mathcal{V}^\mathsf{T}.$$

The singular values of A are simply the eigenvalues of the matrices AA^T and $A^\mathsf{T}A$ and the orthogonal matrices $\mathcal{U}$ and $\mathcal{V}$ the corresponding orthonormal eigenvectors.

From the singular value decomposition -and its connection to the eigenvalue decomposition- we can give another characterisation of the singular values:

$$s_k = \max_{\substack{V_k \subset \mathbb{R}^n \\ \dim V_k = k}} \min_{x \in V_k} \frac{\|Ax\|_2}{\|x\|_2}. \tag{1.1.1}$$

From the SVD, it is possible to directly read the rank of the matrix A. It is simply the number of nonzero singular values.

Singular values are also related to the Frobenius norm of the matrix. In an abuse of notation, viewing A as an element of the vector space $\mathbb{R}^{mn}$, we have by the SVD that

$$A_{ij} = \sum_{k=1}^{r_A} s_k u_{ik} v_{jk} \Rightarrow A = \sum_{k=1}^{r_A} s_k u_k \otimes v_k.$$

Since the vectors (u_k) and (v_k) are orthonormal, it is also the case for $(u_k \otimes v_k)$ thus

$$\|A\|_F^2 = \sum_{k=1}^{r_A} s_k^2.$$

Another important property of the singular value decomposition for the low-rank approximation problem is the following.

Theorem 1.1.2 (Best rank r approximation of a matrix [Sch08])**.** *Let $A \in \mathbb{R}^{m\times n}$ be a matrix and $(U, \Sigma, V^\mathsf{T})$ an SVD of A. The best rank-r of A in the Frobenius norm is given by*

$$A_r = U_r \Sigma_r V_r^\mathsf{T} = \sum_{k=1}^{r} s_k u_k v_k^\mathsf{T},$$

where $U_r \in \mathbb{R}^{m\times r}$, $\Sigma_r \in \mathbb{R}^{r\times r}$ and $V_r \in \mathbb{R}^{n\times r}$ are the respective truncations of U, Σ and V. The error is given by

$$\|A - A_r\|_F = \Big(\sum_{k \geq r+1} s_k^2 \Big)^{1/2}. \tag{1.1.2}$$

The best approximation is unique if $s_r > s_{r+1}$.

Proof. An upper bound is obtained by a direct computation

$$\|A - A_r\|_F^2 = \Big\| \sum_{j \geq r+1} s_j u_j v_j^{\mathsf{T}} \Big\|_F^2 = \Big\| \sum_{j \geq r+1} s_j u_j \otimes v_j \Big\|_2^2 = \sum_{j \geq r+1} s_j^2.$$

The lower bound is shown using a bound on the singular values: let $M, N \in \mathbb{R}^{p \times q}$

$$\forall\, 1 \leq i, j \leq \min(p,q), 0 \leq j \leq d - i, s_{i+j-1}(M+N) \leq s_i(M) + s_j(N), \tag{1.1.3}$$

where $(s_k(M))_k, (s_k(N))_k, (s_k(M+N))_k$ are the respective singular values of M, N and $M+N$. This singular value bounds are derived by considering the following subspaces (without loss of generality, we can assume that $q \leq p$):

$$V^{M+N} = \operatorname{Span}\big(v_1^{M+N}, \dots, v_{i+j-1}^{M+N}\big), \quad V^M = \operatorname{Span}\big(v_i^M, \dots, v_q^M\big)$$
$$V^N = \operatorname{Span}\big(v_j^N, \dots, v_q^N\big).$$

By estimating the dimension of the intersection (by using that $\dim V^M + \dim V^N + \dim V^{M+N} = (q-i+1) + (q-j+1) + i + j - 1 = 2q+1$), we deduce that there exists a normalised vector $x \in V^M \cap V^N \cap V^{M+N}$:

$$s_{i+j-1}(M+N) \leq \|(M+N)x\|_2 \leq \|Mx\|_2 + \|Nx\|_2 \leq s_i(M) + s_j(N).$$

Let $\widetilde{A}_r$ be a matrix of rank r. We apply the inequality (1.1.3) with $M = A - \widetilde{A}_r$, $N = \widetilde{A}_r$ and $j = r+1$. Since $s_{r+1}(\widetilde{A}_r) = 0$, we have

$$\forall\, 1 \leq i \leq q, s_{r+i}(A) \leq s_i(A - \widetilde{A}_r).$$

Hence $\|A - \widetilde{A}_r\|_F^2 = \sum_{i=1}^q s_i(A - \widetilde{A}_r)^2 \geq \sum_{i=r+1}^q s_i(A)^2$, which is the result. □

Remark 1.1.3. *A similar approximation result can be written in the matrix norm $\|\cdot\|_2$ subordinate to the vector $\|\cdot\|_2$. In that case, it is straightforward to check that $\|A - A_r\|_2 = \big\|\sum_{j \geq r+1} s_j u_j v_j^{\mathsf{T}}\big\|_2 = s_{r+1}$. Moreover for a rank-$r$ matrix $\widetilde{A}_r$, by definition, there is a normalised vector $x \in \operatorname{Span}(v_1, \dots, v_{r+1})$ such that $\widetilde{A}_r x = 0$. Thus*

$$\|A - \widetilde{A}_r\|_2 \geq \|(A - \widetilde{A}_r)x\|_2 \geq \|Ax\|_2 \geq s_{r+1}.$$

Another way to phrase the best rank r approximation of a matrix is to take the subspace point of view. A matrix $A \in \mathbb{R}^{m \times n}$ can be viewed as a vector of the product space $\mathbb{R}^m \otimes \mathbb{R}^n$ which is isometrically isomorphic to $\mathbb{R}^{mn}$. The subspace problem is phrased as follows: find subspaces $\mathcal{U} \subset \mathbb{R}^m$ and $\mathcal{V} \subset \mathbb{R}^n$ both of dimension r such that it minimises the distance

$$\operatorname{dist}(A, \mathcal{U} \otimes \mathcal{V}) = \|A - \Pi_{\mathcal{U} \otimes \mathcal{V}} A\| = \min_{\substack{\widetilde{\mathcal{U}} \subset \mathbb{R}^m, \dim \widetilde{\mathcal{U}} = r \\ \widetilde{\mathcal{V}} \subset \mathbb{R}^n, \dim \widetilde{\mathcal{V}} = r}} \|A - \Pi_{\widetilde{\mathcal{U}} \otimes \widetilde{\mathcal{V}}} A\|, \tag{1.1.4}$$

where $\Pi_{\mathcal{W}}$ is the orthogonal projection onto the subspace $\mathcal{W} \subset \mathbb{R}^{mn}$. The SVD gives a characterisation of the solution to the minimisation problem (1.1.4).

Proposition 1.1.4. *Let $A \in \mathbb{R}^{m\times n}$, (U,Σ,V^T) its SVD and $r \in \mathbb{N}$. Denote $(u_1,\dots,u_{r_A})$ and $(v_1,\dots,v_{r_A})$ the respective columns of U and V. A solution to the subspace minimisation problem (1.1.4) is given by*

$$\mathcal{U} = \mathrm{Span}(u_1,\dots,u_r), \quad \mathcal{V} = \mathrm{Span}(v_1,\dots,v_r). \tag{1.1.5}$$

The solution is unique if $s_r > s_{r+1}$.

Proof. Let $\widetilde{\mathcal{U}}$ and $\widetilde{\mathcal{V}}$ be respectively subspaces of $\mathbb{R}^m$ and $\mathbb{R}^n$ of dimension r. Let $(\widetilde{u}_i)_{1\le i\le r}$ and $(\widetilde{v}_i)_{1\le i\le r}$ be ONB of respectively $\widetilde{\mathcal{U}}$ and $\widetilde{\mathcal{V}}$. The minimisation problem (1.1.4) can be rewritten as

$$\min_{\substack{\widetilde{\mathcal{U}}\subset\mathbb{R}^m,\dim\widetilde{\mathcal{U}}=r\\ \widetilde{\mathcal{V}}\subset\mathbb{R}^n,\dim\widetilde{\mathcal{V}}=r}} \|A-\Pi_{\widetilde{\mathcal{U}}\otimes\widetilde{\mathcal{V}}}A\| = \min_{\substack{\widetilde{\mathcal{U}}\subset\mathbb{R}^m,\dim\widetilde{\mathcal{U}}=r\\ \widetilde{\mathcal{V}}\subset\mathbb{R}^n,\dim\widetilde{\mathcal{V}}=r}} \|A-P_{\widetilde{\mathcal{U}}}AP_{\widetilde{\mathcal{V}}}\|_F^2,$$

where $P_{\widetilde{\mathcal{U}}}$ (resp. $P_{\widetilde{\mathcal{V}}}$) is the orthogonal projection onto $\widetilde{\mathcal{U}}$ (resp. $\widetilde{\mathcal{V}}$).

Let $\widetilde{\mathcal{U}}$ and $\widetilde{\mathcal{V}}$ be respectively subspaces of $\mathbb{R}^m$ and $\mathbb{R}^n$ of dimension r. Let $(\widetilde{u}_i)_{1\le i\le r}$ and $(\widetilde{v}_i)_{1\le i\le r}$ be ONB of respectively $\widetilde{\mathcal{U}}$ and $\widetilde{\mathcal{V}}$. Then we have

$$\begin{aligned}\|A-P_{\widetilde{\mathcal{U}}}AP_{\widetilde{\mathcal{V}}}\|_F^2 &= \mathrm{Tr}\big((A-P_{\widetilde{\mathcal{U}}}AP_{\widetilde{\mathcal{V}}})^\mathsf{T}(A-P_{\widetilde{\mathcal{U}}}AP_{\widetilde{\mathcal{V}}})\big)\\ &= \mathrm{Tr}\big(A^\mathsf{T}A - P_{\widetilde{\mathcal{V}}}A^\mathsf{T}P_{\widetilde{\mathcal{U}}}A - A^\mathsf{T}P_{\widetilde{\mathcal{U}}}AP_{\widetilde{\mathcal{V}}} + P_{\widetilde{\mathcal{V}}}A^\mathsf{T}P_{\widetilde{\mathcal{U}}}AP_{\widetilde{\mathcal{V}}}\big)\\ &= \mathrm{Tr}\big(A^\mathsf{T}A\big) - \mathrm{Tr}\big(P_{\widetilde{\mathcal{V}}}A^\mathsf{T}P_{\widetilde{\mathcal{U}}}AP_{\widetilde{\mathcal{V}}}\big),\end{aligned}$$

where we have used that since $P_{\widetilde{\mathcal{V}}}$ is an orthogonal projection, we have $\mathrm{Tr}\big(P_{\widetilde{\mathcal{V}}}A^\mathsf{T}P_{\widetilde{\mathcal{U}}}A\big) = \mathrm{Tr}\big(A^\mathsf{T}P_{\widetilde{\mathcal{U}}}AP_{\widetilde{\mathcal{V}}}\big) = \mathrm{Tr}\big(P_{\widetilde{\mathcal{V}}}A^\mathsf{T}P_{\widetilde{\mathcal{U}}}AP_{\widetilde{\mathcal{V}}}\big)$. We realise that

$$\mathrm{Tr}\big(P_{\widetilde{\mathcal{V}}}A^\mathsf{T}P_{\widetilde{\mathcal{U}}}AP_{\widetilde{\mathcal{V}}}\big) = \sum_{1\le i,j\le r} \big|\langle \widetilde{u}_i, A\widetilde{v}_j\rangle\big|^2.$$

Solving the minimisation problem (1.1.4) is equivalent to maximising $\sum_{1\le i,j\le r}\big|\langle\widetilde{u}_i,A\widetilde{v}_j\rangle\big|^2$ where $(\widetilde{u}_i)_{1\le i\le r}$ and $(\widetilde{v}_i)_{1\le i\le r}$ are orthonormal families. Using the max-min characterisation of the singular values (1.1.1), we have $\sum_{1\le i,j\le r}\big|\langle\widetilde{u}_i,A\widetilde{v}_j\rangle\big|^2 \le \sum_{j=1}^r\|A\widetilde{v}_j\|^2 \le \sum_{j=1}^r s_j^2$. The upper bound is attained for $\widetilde{\mathcal{U}} = \mathrm{Span}(u_1,\dots,u_r)$ and $\widetilde{\mathcal{V}} = \mathrm{Span}(v_1,\dots,v_r)$. □

1.1.2 Generalisations of the SVD for tensors

A tensor $\boldsymbol{u}$ of order $d\in\mathbb{N}$ is a multidimensional array $(\boldsymbol{u}_{i_1\dots i_d}) \in \mathbb{R}^{n_1\times\cdots\times n_d}$.

For higher-order tensors, different generalisations of the SVD are possible. With the previous discussion, there are two natural options that emerge:

- write the tensor as a sum of rank-1 tensors:

$$\boldsymbol{u} = \sum_{\alpha=1}^r u_\alpha^{(1)}\otimes\cdots\otimes u_\alpha^{(d)},$$

where for all $k \in [\![d]\!]$, $u_\alpha^{(k)} \in \mathbb{R}^{n_k}$. This is the *canonical polyadic decomposition* (CP decomposition);

- consider the subspace minimisation problem:

$$\operatorname{dist}(\boldsymbol{u}, \mathcal{U}_1 \otimes \mathcal{U}_2 \otimes \cdots \otimes \mathcal{U}_d) = \min_{\widetilde{\mathcal{U}}_1 \subset \mathbb{R}^{n_1}, \dim \widetilde{\mathcal{U}}_1 = r_1, \ldots, \widetilde{\mathcal{U}}_d \subset \mathbb{R}^{n_d}, \dim \widetilde{\mathcal{U}}_d = r_d} \|\boldsymbol{u} - \Pi_{\widetilde{\mathcal{U}}_1 \otimes \cdots \otimes \widetilde{\mathcal{U}}_d} \boldsymbol{u}\|,$$

where $\dim \mathcal{U}_k = r_k$ for all $k \in [\![d]\!]$. This yields the Tucker decomposition.

The canonical decomposition looks the most appealing as it is the most sparse way to represent a tensor. It has however one major drawback, being that the best rank r approximation (in the sense of the CP decomposition) is *ill-posed!* [DSL08] Consider noncolinear vectors $a \in \mathbb{R}^n$, $b \in \mathbb{R}^n$ and the tensor

$$\boldsymbol{u} = b \otimes a \otimes a + a \otimes b \otimes a + a \otimes a \otimes b.$$

which is a tensor of canonical rank 3. It can however be approximated as well as we wish by a tensor of canonical rank 2: let $\varepsilon > 0$, then we see that

$$\boldsymbol{u} - \left(\frac{1}{\varepsilon}(a + \varepsilon b) \otimes (a + \varepsilon b) \otimes (a + \varepsilon b) - \frac{1}{\varepsilon} a \otimes a \otimes a \right) = \mathcal{O}(\varepsilon). \tag{1.1.6}$$

This example highlights that the set of tensors of canonical rank less than 2 is not closed. Contrary to matrices, the set of tensors of canonical rank less than r is not closed.

Regarding the Tucker decomposition, let $\boldsymbol{u} \in \mathcal{U}_1 \otimes \cdots \otimes \mathcal{U}_d$. Then there is a core tensor $\boldsymbol{c} \in \mathbb{R}^{r_1 \times \cdots \times r_d}$ and matrices $(U_k)_{1 \leq k \leq d} \in \bigotimes_{k=1}^d \mathbb{R}^{n_k \times r_k}$ such that

$$\forall\, \mathbf{i} \in [\![\mathbf{n}]\!],\ \boldsymbol{u}_{i_1 \ldots i_d} = \sum_{\alpha_1=1}^{r_1} \cdots \sum_{\alpha_d=1}^{r_d} \boldsymbol{c}_{\alpha_1 \ldots \alpha_d} (U_1)_{i_1}^{\alpha_1} \cdots (U_d)_{i_d}^{\alpha_d}.$$

The storage cost of the tensor $\boldsymbol{u}$ is still exponential in the order d of the tensor (except if some r_k are equal to 1). As such it is a useful decomposition only for low order tensors. In the following, we will focus on the efficient representation of tensors of order up to a hundred, for which the Tucker decomposition is not suited.

1.2 Tensor train decomposition

1.2.1 Hierarchical SVD and tensor trains

We first define the reshape of a tensor.

Definition 1.2.1 (Reshape of a tensor)**.** *Let $\boldsymbol{u} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$ be a tensor. Let $\ell \in [\![d]\!]$. We say that the matrix $\left(\boldsymbol{u}_{i_1 \ldots i_\ell ; i_{\ell+1} \ldots i_d}\right) \in \mathbb{R}^{n_1 \cdots n_\ell \times n_{\ell+1} \cdots n_d}$ is a reshape of $\boldsymbol{u}$ with respect to the modes $[\![\ell]\!]$. This reshape will be denoted by $\boldsymbol{u}^{\leq \ell}$ and for $\mathbf{i} \in [\![\mathbf{n}]\!]$ its elements $\boldsymbol{u}_{i_1 \ldots i_\ell}^{i_{\ell+1} \ldots i_d}$.*

The reshapes $\boldsymbol{u}^{\leq \ell}$ for $1 \leq \ell \leq d-1$ will be of particular interest.

To derive a tensor decomposition generalising the SVD, one can apply the SVD successively. Let $\boldsymbol{u} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$ be a tensor and proceed as follows (we use here Einstein convention where we sum over repeated indices)

$$\begin{aligned}
\boldsymbol{u}_{i_1 \dots i_d} &= (\boldsymbol{u}_{i_1}^{i_2 \dots i_d}) && \text{(reshape of } \boldsymbol{u} \text{ to } n_1 \times n_2 \cdots n_d) \\
&= (U_1)_{i_1}^{\alpha_1} (\Sigma_1 V_1^{\mathsf{T}})_{\alpha_1}^{i_2 \dots i_d} && \text{(SVD)} \\
&= (U_1)_{i_1}^{\alpha_1} (\Sigma_1 V_1^{\mathsf{T}})_{\alpha_1 i_2}^{i_3 \dots i_d} && \text{(reshape of } \Sigma_1 V_1^{\mathsf{T}}) \\
&= (U_1)_{i_1}^{\alpha_1} (U_2)_{\alpha_1 i_2}^{\alpha_2} (\Sigma_2 V_2^{\mathsf{T}})_{\alpha_2}^{i_3 \dots i_d} && \text{(SVD of } \Sigma_1 V_1^{\mathsf{T}}) \\
&= (U_1)_{i_1}^{\alpha_1} (U_2)_{\alpha_1 i_2}^{\alpha_2} (\Sigma_2 V_2^{\mathsf{T}})_{\alpha_2 i_3}^{i_4 \dots i_d} && \text{(reshape of } \Sigma_2 V_2^{\mathsf{T}}),
\end{aligned}$$

where we repeat the process until we get

$$\boldsymbol{u}_{i_1 \dots i_d} = (U_1)_{i_1}^{\alpha_1} (U_2)_{\alpha_1 i_2}^{\alpha_2} \cdots (U_{d-1})_{\alpha_{d-2} i_{d-1}}^{\alpha_{d-1}} (\Sigma_{d-1} V_{d-1}^{\mathsf{T}})_{\alpha_{d-1}}^{i_d}.$$

The tensors appearing in the decomposition above can be rearranged as below

$$\begin{aligned}
\boldsymbol{u}_{i_1 \dots i_d} &= (U_1)_{i_1}^{\alpha_1} \quad (U_2)_{\alpha_1 i_2}^{\alpha_2} \quad \cdots \quad (U_{d-1})_{\alpha_{d-2} i_{d-1}}^{\alpha_{d-1}} (\Sigma_{d-1} V_{d-1}^{\mathsf{T}})_{\alpha_{d-1}}^{i_d} \\
&= A_1[i_1]_{\alpha_1} \quad A_2[i_2]_{\alpha_2}^{\alpha_1} \quad \cdots \quad A_{d-1}[i_{d-1}]_{\alpha_{d-1}}^{\alpha_{d-2}} \quad A_d[i_d]^{\alpha_{d-1}}.
\end{aligned}$$

The decomposition above is called the *tensor train* (TT) decomposition [OT09], also called *matrix product state* [KSZ91] in the physics litterature is the simplest instance of a tensor network. This terminology will be clearer when the graphical representations of the tensor formats will be presented in Section 2.1.1.

Definition 1.2.2 ([KSZ91, OT09]). *Let $\boldsymbol{u} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$ be a tensor. We say that $(A_1, \dots, A_d)$ is a tensor train decomposition of $\boldsymbol{u}$ if we have for all $\mathbf{i} \in [\![\mathbf{n}]\!]$*

$$\begin{aligned}
\boldsymbol{u}_{i_1 \dots i_d} &= A_1[i_1] A_2[i_2] \cdots A_d[i_d] && (1.2.1) \\
&= \sum_{\alpha_1=1}^{r_1} \sum_{\alpha_2=1}^{r_2} \cdots \sum_{\alpha_{d-1}=1}^{r_{d-1}} A_1[i_1]_{\alpha_1} A_2[i_2]_{\alpha_2}^{\alpha_1} \cdots A_d[i_d]^{\alpha_{d-1}}, && (1.2.2)
\end{aligned}$$

where for each $i_k \in [\![n_k]\!]$, $A_k[i_k] \in \mathbb{R}^{r_{k-1} \times r_k}$ ($r_0 = r_d = 1$). The tensor $A_k \in \mathbb{R}^{r_{k-1} \times n_k \times r_k}$ are called the TT cores *and the sizes of the TT cores are the* TT ranks *of $\boldsymbol{u}$.*

Such a representation has a storage cost of $\sum_{k=1}^{d} n_k r_{k-1} r_k$. Provided that the TT ranks do not increase exponentially with the order d of the tensor, the TT decomposition is a sparse representation of the tensor $\boldsymbol{u}$.

An exact TT representation of any tensor can be achieved by the algorithm presented at the beginning of Section 1.2.1 and given in Algorithm 1.1. This algorithm is called the hierarchical SVD (HSVD) [Vid03, OT09].

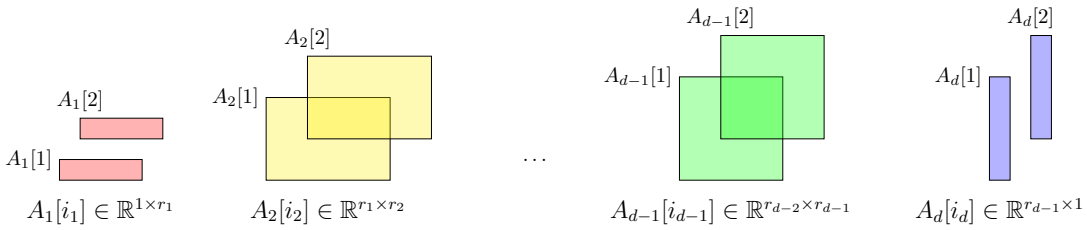


Figure 1.1: Schematic representation of the TT decomposition of a tensor in $\mathbb{R}^{2\times\cdots\times 2}$

It is clear that there is no uniqueness of the TT decomposition. Indeed for a tensor $\boldsymbol{u} \in \mathbb{R}^{n_1\times\cdots\times n_d}$ if $(A_1, \ldots, A_d)$ is a tensor train decomposition, then for any invertible matrices $(G_k)_{1\leq k\leq d-1} \in \bigotimes_{k=1}^{d-1} \mathrm{GL}_{r_k}(\mathbb{R})$, the TT cores $(\widetilde{A}_1, \ldots, \widetilde{A}_d)$ defined by

$$\begin{cases} \widetilde{A}_1[i_1] = A_1[i_1]G_1, \ i_1 \in [\![n_1]\!], \quad \widetilde{A}_d[i_d] = G_{d-1}^{-1}A_d[i_d], \ i_d \in [\![n_d]\!] \\ \widetilde{A}_k[i_k] = G_{k-1}^{-1}A_k[i_k]G_k, \ i_k \in [\![n_k]\!], \ k \in [\![2; d-1]\!], \end{cases}$$

is an equivalent TT representation. It is possible to partially lift this gauge freedom. This discussion is postponed to Section 1.2.5.

The history of the TT decomposition dates back to the density-matrix renormalisation group (DMRG) [Whi92] pioneered by White for the computation of properties of one-dimensional statistical physics systems. The connection between DMRG and TT has been realised later [OR95, DMNS98].

Example 1.2.3.

- *a tensor product* $\boldsymbol{u}_{i_1\ldots i_d} = u_{i_1}^{(1)} \cdots u_{i_d}^{(d)}$ *is a TT of TT rank 1, as the cores are* $(u_{i_k}^{(k)})_{1\leq k\leq d, 1\leq i_k\leq n_k}$.

- *the unnormalised Bell state* $\boldsymbol{b} \in \bigotimes_1^{2d} \mathbb{R}^2$

$$\boldsymbol{b}_{i_1\ldots i_{2d}} = \big(\delta_{1,i_1}\delta_{2,i_2} + \delta_{2,i_1}\delta_{1,i_2}\big)\big(\delta_{1,i_3}\delta_{2,i_4} + \delta_{2,i_3}\delta_{1,i_4}\big)\cdots\big(\delta_{1,i_{2d-1}}\delta_{2,i_{2d}} + \delta_{2,i_{2d-1}}\delta_{1,i_{2d}}\big),$$

is a TT of rank 2: let $(B_k)_{1\leq k\leq 2d}$ *be defined by*

$$B_{2k-1}[i_{2k-1}] = \begin{bmatrix}\delta_{1i_{2k-1}} & \delta_{2i_{2k-1}}\end{bmatrix}, \quad B_{2k}[i_{2k}] = \begin{bmatrix}\delta_{2i_{2k}} \\ \delta_{1i_{2k}}\end{bmatrix}, \quad k = 1, \ldots, d. \tag{1.2.3}$$

By a direct calculation, we can check that $\boldsymbol{b}_{i_1\ldots i_{2d}} = B_1[i_1]\cdots B_{2d}[i_d]$.

- *for* $d = 2$, *the following reordering of the indices of the Bell state* $\widetilde{\boldsymbol{b}} \in \bigotimes_1^4 \mathbb{R}^2$

$$\widetilde{\boldsymbol{b}}_{i_1\ldots i_4} = \big(\delta_{1,i_1}\delta_{2,i_3} + \delta_{2,i_1}\delta_{1,i_3}\big)\big(\delta_{1,i_2}\delta_{2,i_4} + \delta_{2,i_3}\delta_{1,i_4}\big)$$

has a TT decomposition of rank 4:

i_k	$\widetilde{B}_1$	$\widetilde{B}_2$	$\widetilde{B}_3$	$\widetilde{B}_4$
1	$\begin{bmatrix}1 & 0\end{bmatrix}$	$\begin{bmatrix}1 & 0 & 0 & 0\\ 0 & 0 & 1 & 0\end{bmatrix}$	$\begin{bmatrix}0 & 0\\ 0 & 0\\ 1 & 0\\ 0 & 1\end{bmatrix}$	$\begin{bmatrix}0\\ 1\end{bmatrix}$
2	$\begin{bmatrix}0 & 1\end{bmatrix}$	$\begin{bmatrix}0 & 1 & 0 & 0\\ 0 & 0 & 0 & 1\end{bmatrix}$	$\begin{bmatrix}1 & 0\\ 0 & 1\\ 0 & 0\\ 0 & 0\end{bmatrix}$	$\begin{bmatrix}1\\ 0\end{bmatrix}$

This elementary example highlights the importance of the ordering of the indices of the tensor for an efficient TT representation. The TT decomposition above can be derived by using that $(AC)\otimes(BD) = (A\otimes B)(C\otimes D)$ *for matrices with compatible sizes. Hence the formula for the TT cores of the reordered Bell state is obtained from the TT decomposition* (1.2.3) *of the Bell state*

$$\begin{aligned}\widetilde{\boldsymbol{b}}_{i_1i_2i_3i_4} = \boldsymbol{b}_{i_1i_3i_2i_4} &= B_1[i_1]B_2[i_3]B_3[i_2]B_4[i_4]\\ &= B_1[i_1](\mathrm{id}_2\, B_2[i_3]\otimes B_3[i_2]\,\mathrm{id}_2)B_4[i_4]\\ &= B_1[i_1](\mathrm{id}_2\otimes B_3[i_2])(B_2[i_3]\otimes \mathrm{id}_2)B_4[i_4].\end{aligned}$$

Remark 1.2.4. *The reordered Bell state example* $\widetilde{\boldsymbol{b}} \in \bigotimes_1^{2d}\mathbb{R}^2$

$$\widetilde{\boldsymbol{b}}_{i_1\dots i_{2d}} = \prod_{k=1}^{d}\left(\delta_{1,i_k}\delta_{2,i_{k+d}} + \delta_{2,i_k}\delta_{1,i_{k+d}}\right)$$

has a TT decomposition of rank 2^d*. The optimality of the ranks is proved by the characterisation of the TT ranks stated in Theorem 1.2.12.*

The central tool in the TT decomposition is the HSVD presented earlier and summarised in Algorithm 1.1. From the characterisation of the error in the truncated SVD, it is expected that the HSVD can be used to derive an approximation result by a TT with given TT ranks. This will be treated in Section 1.2.4.

Remark 1.2.5. *It is reasonably clear that such an algorithm extends to the decomposition into a tree tensor network. Indeed, in the HSVD algorithm, we simply partition* $\{1,\dots,d\}$ *into the sets* $(\{1\},\{2,\dots,d\})$*, then* $(\{1\},\{2\},\{3,\dots,d\})$*, and so on so forth. For trees, we choose different partition choices that does not have to reduce to a singleton right away. For tensor networks with loops, there is no equivalent of the HSVD for the construction of a tensor network directly from the tensor. This makes the analysis of such networks much more difficult.*

Algorithm 1.1 Hierarchical SVD

Input: Tensor $\boldsymbol{u} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$
Output: $(A_1, \ldots, A_d)$ TT representation of $\boldsymbol{u}$

function HSVD($\boldsymbol{u}$)
  $T_{\alpha_0 i_1}^{i_2 \ldots i_d} = \boldsymbol{u}_{i_1}^{i_2 \ldots i_d}$ (α_0 dummy index)
  for $k = 1, \ldots, d-1$ **do**
    $U_k, \Sigma_k, V_k^{\mathsf{T}} = \mathtt{svd}\left(T_{\alpha_{k-1} i_k}^{i_{k+1} \ldots i_d}\right)$
    $A_k[i_k]_{\alpha_{k-1}}^{\alpha_k} = (U_k)_{\alpha_{k-1} i_k}^{\alpha_k}$
    $T_{\alpha_k i_{k+1}}^{i_{k+2} \ldots i_d} = \left(\Sigma_k V_k^{\mathsf{T}}\right)_{\alpha_k}^{i_{k+1} i_{k+2} \ldots i_d}$
  end for
  $A_d[i_d]^{\alpha_{d-1}} = \left(\Sigma_{d-1} V_{d-1}^{\mathsf{T}}\right)_{\alpha_{d-1}}^{i_d}$
  return $(A_1, \ldots, A_d)$
end function

1.2.2 Algebraic properties of TT and normalisation of TT

The TT decomposition has reasonable algebraic properties as it is stable by multiplication by a scalar and by addition -up to augmentation of the TT ranks.

Proposition 1.2.6 (Algebraic properties of TT)**.** *Let $(A_1, \ldots, A_d)$ and $(\widetilde{A}_1, \ldots, \widetilde{A}_d)$ be the respective TT decompositions of the tensors $\boldsymbol{u}, \widetilde{\boldsymbol{u}} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$. Let $\lambda \in \mathbb{R}$. Then*

- *$\lambda \boldsymbol{u}$ has a TT decomposition given by $(B_k)_{k \in [\![d]\!]}$ with $B_k = A_k$ for $k \in [\![d-1]\!]$ and $B_d = \lambda A_d$;*
- *the sum $\boldsymbol{u} + \widetilde{\boldsymbol{u}}$ has a TT decomposition $(S_k)_{k \in [\![d]\!]}$ given by*

$$\begin{aligned} S_1[i_1] &= \begin{bmatrix} A_1[i_1] & \widetilde{A}_1[i_1] \end{bmatrix}, \quad S_d[i_d] = \begin{bmatrix} A_d[i_d] \\ \widetilde{A}_d[i_d] \end{bmatrix} \\ S_k[i_k] &= \begin{bmatrix} A_k[i_k] & 0 \\ 0 & \widetilde{A}_k[i_k] \end{bmatrix}, k \in [\![2; d-1]\!]. \end{aligned} \tag{1.2.4}$$

The first item is clear and the proof for the sum consists in expanding the TT decomposition $(S_1, \ldots, S_d)$. The TT decomposition of the sum (1.2.4) is in general not minimal and can be compressed as explained in Section 1.2.4.

Remark 1.2.7. *Since a tensor product $u^{(1)} \otimes \cdots \otimes u^{(d)}$ is a TT of rank 1, we deduce that a CP decomposition of rank r has at most a TT representation of rank r. The TT decomposition is a generalisation of the CP format, with advantageous algebraic and topologic properties.*

The TT decomposition can be seen as a structured low-rank representation of a tensor $\boldsymbol{u} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$. Indeed, if $(A_1, \ldots, A_d)$ is a TT representation of $\boldsymbol{u}$, for any $k \in [\![d-1]\!]$, we can write

$$\boldsymbol{u}^{\leq k} = \underbrace{\begin{bmatrix} A_1[1]A_2[1]\cdots A_k[1] \\ \vdots \\ A_1[n_1]A_2[n_2]\cdots A_k[n_k] \end{bmatrix}}_{\in \mathbb{R}^{n_1 \cdots n_k \times r_k}} \underbrace{\begin{bmatrix} A_{k+1}[1] & \cdots & A_d[1] & \ldots & A_{k+1}[n_{k+1}] & \cdots & A_d[n_d] \end{bmatrix}}_{\in \mathbb{R}^{r_k \times n_{k+1} \cdots n_d}},$$

which is a rank-r_k matrix decomposition of the reshape $\boldsymbol{u}^{\leq k} \in \mathbb{R}^{n_1 \cdots n_k \times n_{k+1} \cdots n_d}$. This observation will be used in the next sections.

The TT cores $(A_k)_{k \in [\![d]\!]}$ obtained from the HSVD algorithm satisfy a particular property. From the definition of the SVD, we have that the reshaped TT core $((A_k)^{\alpha_k}_{i_k \alpha_{k-1}}) \in \mathbb{R}^{n_k r_{k-1} \times r_k}$ is a partial isometry for any $k \in [\![d-1]\!]$, *i.e.* we have $((A_k)^{\alpha_k}_{i_k \alpha_{k-1}})^{\mathsf{T}}((A_k)^{\alpha_k}_{i_k \alpha_{k-1}}) = \mathrm{id}_{r_k}$. We say in that case that are *left-orthogonal* or *left-normalised.*

Definition 1.2.8 (TT normalisation)**.** *Let $(A_k)_{k \in [\![d]\!]}$ be a TT decomposition of a tensor $\boldsymbol{u} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$ with TT ranks $(r_k)_{k \in [\![0;d]\!]}$. Let $\ell \in [\![d]\!]$. We say that a TT decomposition $(A_1, \ldots, A_d)$ is* ℓ-normalised *or* normalised with root ℓ *if for all $k \in [\![\ell - 1]\!]$*

$$\sum_{i_k=1}^{n_k} A_k[i_k]^{\mathsf{T}} A_k[i_k] = \mathrm{id}_{r_k};$$

and for all $k \in [\![\ell + 1; d]\!]$

$$\sum_{i_k=1}^{n_k} A_k[i_k] A_k[i_k]^{\mathsf{T}} = \mathrm{id}_{r_{k-1}}.$$

If $\ell = 1$, we say that $(A_k)_{k \in [\![d]\!]}$ is left-orthogonal *or* left-normalised*. If $\ell = d$, we say that $(A_k)_{k \in [\![d]\!]}$ is* right-orthogonal *or* right-normalised*.*

The HSVD algorithm described in Algorithm 1.1 yields a left-orthogonal TT decomposition of the tensor $\boldsymbol{u}$. This is because successive SVDs are performed starting from the first index of the tensor $\boldsymbol{u}$. By performing successive SVDs from the "right", *i.e.* by first doing the SVD of $\boldsymbol{u}^{\leq d-1} \in \mathbb{R}^{n_1 \cdots n_{d-1} \times n_d} = (U_{d-1}\Sigma_{d-1})^{\alpha_{d-1}}_{i_1 \ldots i_{d-1}} (V^{\mathsf{T}}_{d-1})^{i_d}_{\alpha_{d-1}}$, then the SVD of $(U_{d-1}\Sigma_{d-1})^{i_{d-1}\alpha_{d-1}}_{i_1 \ldots i_{d-2}}$ and so on and so forth, one would get a right-orthogonal TT representation of $\boldsymbol{u}$.

TT representations with a specific normalisation have convenient properties.

Proposition 1.2.9. *Let $(A_k)_{k \in [\![d]\!]}$ be a left-orthogonal TT decomposition of a tensor $\boldsymbol{u}\mathbb{R}^{n_1 \times \cdots \times n_d}$ with TT ranks $(r_k)_{k \in [\![0;d]\!]}$. Then we have that*

- $\|\boldsymbol{u}\| = \|A_d\|$;

- *for any $k \in [\![d-1]\!]$, we have that the matrix*

$$\begin{bmatrix} A_1[1]A_2[1]\cdots A_k[1] \\ \vdots \\ A_1[n_1]A_2[n_2]\cdots A_k[n_k] \end{bmatrix} \in \mathbb{R}^{n_1\cdots n_k \times r_k}$$

is a partial isometry.

Proof. For any $k \in [\![d-1]\!]$ we have

$$\begin{aligned}
&\begin{bmatrix} A_1[1]A_2[1]\cdots A_k[1] \\ \vdots \\ A_1[n_1]A_2[n_2]\cdots A_k[n_k] \end{bmatrix}^{\mathsf{T}} \begin{bmatrix} A_1[1]A_2[1]\cdots A_k[1] \\ \vdots \\ A_1[n_1]A_2[n_2]\cdots A_k[n_k] \end{bmatrix} \\
&\qquad = \sum_{i_1=1}^{n_1} \cdots \sum_{i_k=1}^{n_k} (A_k[i_k])^{\mathsf{T}} A_1[i_1]^{\mathsf{T}} \cdots A_1[i_1] \cdots A_k[i_k] \\
&\qquad = \sum_{i_2=1}^{n_2} \cdots \sum_{i_k=1}^{n_k} A_k[i_k]^{\mathsf{T}} \cdots A_2[i_2]^{\mathsf{T}} \Big(\underbrace{\sum_{i_1=1}^{n_1} A_1[i_1]^{\mathsf{T}} A_1[i_1]}_{=\mathrm{id}_{r_1}} \Big) A_2[i_2] \cdots A_k[i_k] \\
&\qquad = \mathrm{id}_{r_k},
\end{aligned}$$

by left-orthogonality of the TT cores.

For the norm, we have

$$\|\boldsymbol{u}\| = \|\boldsymbol{u}^{\leq d}\| = \left\| \underbrace{\begin{bmatrix} A_1[1]A_2[1]\cdots A_{d-1}[1] \\ \vdots \\ A_1[n_1]A_2[n_2]\cdots A_{d-1}[n_{d-1}] \end{bmatrix}}_{\in \mathbb{R}^{n_1\cdots n_{d-1}\times r_{d-1}}} \underbrace{\begin{bmatrix} A_d[1] & \ldots & A_d[n_d] \end{bmatrix}}_{\in \mathbb{R}^{r_{d-1}\times n_d}} \right\| = \|A_d\|,$$

as the first matrix is a partial isometry. □

It is convenient to introduce the $\bowtie$ notation, which simplifies the manipulation of expressions involving partial contractions of tensors of order 3.

Definition 1.2.10 (Strong Kronecker product)**.** *For $(B, C) \in \mathbb{R}^{r\times n\times \tilde{r}} \times \mathbb{R}^{\tilde{r}\times \tilde{n}\times \hat{r}}$, the strong Kronecker product denoted by $B \bowtie C \in \mathbb{R}^{r\times n\times \tilde{n}\times \hat{r}}$, is defined by*

$$(B \bowtie C)_{\alpha j \tilde{j} \hat{\alpha}} = \sum_{\tilde{\alpha}=1}^{\tilde{r}} B_{\alpha j \tilde{\alpha}} C_{\tilde{\alpha}\tilde{j}\hat{\alpha}}.$$

Proposition 1.2.11. *Let $(A_k)_{k\in[\![d]\!]}$ is a TT representation of a tensor $\boldsymbol{u}$. Then we have*

(i). $\boldsymbol{u} = A_1 \bowtie \ldots \bowtie A_d$;

(ii). *for any $k \in [\![d-1]\!]$, we have that* $\boldsymbol{u}^{\leq k} = (A_1 \bowtie \ldots \bowtie A_k)^{\leq k}(A_{k+1} \bowtie \ldots \bowtie A_d)^{\leq 1}$;

(iii). *if $(A_k)_{k\in[\![d]\!]}$ is a left-orthogonal TT representation of a tensor, then for any $k \in [\![d-1]\!]$, $(A_1 \bowtie \ldots \bowtie A_k)^{\leq k} \in \mathbb{R}^{n_1\cdots n_k \times r_k}$ is a partial isometry.*

1.2.3 Characterisation of exact TT representations

From the hierarchical SVD (Algorithm 1.1), we directly get a characterisation of the TT ranks of the exact TT representation of the tensor.

Theorem 1.2.12 (Characterisation of the TT ranks [HRS12b])**.** *Let $\boldsymbol{u} \in \mathbb{R}^{n_1\times\cdots\times n_d}$ be a tensor. Then the following assertions are true:*

(i). *the minimal TT ranks $(r_1, \ldots, r_{d-1})$ is equal to the rank of the reshapes of $\boldsymbol{u}$,* i.e.

$$\forall k \in [\![d-1]\!], r_k = \operatorname{Rank}(\boldsymbol{u}^{\leq k}).$$

We will thus call $(\operatorname{Rank}(\boldsymbol{u}^{\leq k}))_{k\in[\![d-1]\!]}$ *the* TT ranks *of $\boldsymbol{u}$;*

(ii). *the HSVD algorithm 1.1 gives a TT decomposition of minimal TT ranks.*

This theorem states that the ranks of the optimal TT representation of a tensor $\boldsymbol{u}$ is characterised by its reshapes $(\boldsymbol{u}^{\leq k})_{k[\![d-1]\!]}$. Moreover the HSVD algorithm 1.1 produces a TT representation of $\boldsymbol{u}$ with optimal ranks.

Proof. Let $(\widetilde{A}_1, \ldots, \widetilde{A}_d)$ be a TT representation of $\boldsymbol{u}$ of TT ranks $(\widetilde{r}_k)_{k\in[\![0;d]\!]}$. For any $k \in [\![d-1]\!]$, we have

$$(\boldsymbol{u}^{i_{k+1}\ldots i_d}_{i_1\ldots i_k}) = \underbrace{\begin{bmatrix} \widetilde{A}_1[1]\widetilde{A}_2[1]\cdots\widetilde{A}_k[1] \\ \vdots \\ \widetilde{A}_1[n_1]\widetilde{A}_2[n_2]\cdots\widetilde{A}_k[n_k] \end{bmatrix}}_{\in\mathbb{R}^{n_1\cdots n_k\times\widetilde{r}_k}} \underbrace{\begin{bmatrix} \widetilde{A}_{k+1}[1] & \cdots & \widetilde{A}_d[1] & \ldots & \widetilde{A}_{k+1}[n_{k+1}] & \cdots & \widetilde{A}_d[n_d] \end{bmatrix}}_{\in\mathbb{R}^{\widetilde{r}_k\times n_{k+1}\cdots n_d}}.$$

This shows that any TT representation of $\boldsymbol{u}$ has TT ranks at least $(\operatorname{Rank}(\boldsymbol{u}^{\leq k}))_{k\in[\![0;d]\!]}$.

Let $(A_1, \ldots, A_d)$ be the TT cores given by the HSVD algorithm. Using the same notation as in Algorithm 1.1, for any $k \in [\![d-1]\!]$ we have

$$\boldsymbol{u}^{\leq k} = \underbrace{\begin{bmatrix} A_1[1]A_2[1]\cdots A_k[1] \\ \vdots \\ A_1[n_1]A_2[n_2]\cdots A_k[n_k] \end{bmatrix}}_{\in\mathbb{R}^{n_1\cdots n_k\times r_k}} \Sigma_k V_k^{\mathsf{T}}.$$

The first matrix is a partial isometry by Proposition 1.2.9 hence the equation above is an SVD of $\boldsymbol{u}^{\leq k}$. By the properties of the SVD, we have that $r_k = \operatorname{Rank}(\boldsymbol{u}^{\leq k})$. □

An important consequence of Theorem 1.2.12 is the closedness of the set with prescribed TT ranks.

Proposition 1.2.13. *Let* $\mathbf{r} \in \mathbb{N}^{d+1}$. *The set of tensor trains with TT rank less that* $\mathbf{r}$

$$\mathscr{M}_{\mathrm{TT}_{\leq \mathbf{r}}} = \left\{ \boldsymbol{u} \mid \exists (A_k)_{k \in [\![d]\!]} \in \bigtimes_{k \in [\![d]\!]} \mathbb{R}^{n_k \times r_{k-1} \times r_k},\ \forall\, \mathbf{i} \in [\![\mathbf{n}]\!],\ \boldsymbol{u}_{i_1 \dots i_d} = A_1[i_1] \cdots A_d[i_d] \right\},$$

is a closed set.

Proof. The proof follows from the characterisation of the TT ranks given by Theorem 1.2.12: given a tensor $\boldsymbol{u}$, for $1 \leq k \leq d-1$, the minimal TT rank r_k is equal to the rank of the matrix $\boldsymbol{u}_{i_1 \dots i_k}^{i_{k+1} \dots i_d}$. We conclude by recalling that the set of matrices with rank less than r is a closed set. □

This proposition is in stark contrast with the set of tensors with a given canonical rank r

$$\mathscr{M}_{\mathrm{CP}_{\leq r}} = \left\{ \boldsymbol{u} \mid \forall\, \alpha \in [\![r]\!], \exists\, (v_j^{(\alpha)})_{j \in [\![d]\!]} \in \bigtimes_{j=1}^{d} \mathbb{R}^{n_j}, \boldsymbol{u} = \sum_{\alpha=1}^{r} v_1^{(\alpha)} \otimes \cdots \otimes v_d^{(\alpha)} \right\},$$

as the example exhibited in eq. (1.1.6) shows that the set $\mathscr{M}_{\mathrm{CP}_{\leq r}}$ is not closed if $d \geq 3$ and $r \geq 2$.

Since the set $\mathscr{M}_{\mathrm{TT}_{\leq \mathbf{r}}}$ is closed, we can safely study the question of the best approximation of a tensor with given TT ranks.

1.2.4 Approximation by TT

A natural way to reduce the TT ranks of the TT representation of a tensor is to truncate the SVD at each step of the HSVD algorithm to a tolerance ε:

$$\begin{aligned}
\boldsymbol{u}_{i_1 \dots i_d} &= \boldsymbol{u}_{i_1}^{i_2 \dots i_d} && \text{(reshape of } \boldsymbol{u} \text{ to } n_1 \times n_2 \cdots n_d) \\
&\simeq (U_1)_{i_1}^{\alpha_1} (\Sigma_1^{\varepsilon} V_1^{\mathsf{T}})_{\alpha_1}^{i_2 \dots i_d} && \text{(truncated SVD)} \\
&\simeq (U_1)_{i_1}^{\alpha_1} (\Sigma_1^{\varepsilon} V_1^{\mathsf{T}})_{\alpha_1 i_2}^{i_3 \dots i_d} && \text{(reshape of } \Sigma_1^{\varepsilon} V_1^{\mathsf{T}}) \\
&\simeq (U_1)_{i_1}^{\alpha_1} (U_2)_{\alpha_1 i_2}^{\alpha_2} (\Sigma_2^{\varepsilon} V_2^{\mathsf{T}})_{\alpha_2}^{i_3 \dots i_d} && \text{(truncated SVD of } \Sigma_1^{\varepsilon} V_1^{\mathsf{T}}) \\
&\simeq (U_1)_{i_1}^{\alpha_1} (U_2)_{\alpha_1 i_2}^{\alpha_2} (\Sigma_2^{\varepsilon} V_2^{\mathsf{T}})_{\alpha_2 i_3}^{i_4 \dots i_d} && \text{(reshape of } \Sigma_2^{\varepsilon} V_2^{\mathsf{T}}),
\end{aligned}$$

we repeat the process until we get

$$\boldsymbol{u}_{i_1 \dots i_d} \simeq (U_1)_{i_1}^{\alpha_1} (U_2)_{\alpha_1 i_2}^{\alpha_2} \cdots (U_{d-1})_{\alpha_{d-2} i_{d-1}}^{\alpha_{d-1}} (\Sigma_{d-1}^{\varepsilon} V_{d-1}^{\mathsf{T}})_{\alpha_{d-1}}^{i_d}.$$

Algorithm 1.2 Hierarchical SVD with truncations or TT-SVD

Input: Tensor $\boldsymbol{u} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$, tolerance ε
Output: $(A_1, \dots, A_d)$ TT representation of $\boldsymbol{u}$

function TT-SVD($\boldsymbol{u}, \varepsilon$)
  $T_{\alpha_0 i_1}^{i_2 \dots i_d} = \boldsymbol{u}_{i_1}^{i_2 \dots i_d}$ (α_0 dummy index)
  for $k = 1, \dots, d-1$ **do**
    $U_k, \Sigma_k, V_k^\mathsf{T} = \mathtt{tsvd}\left(T_{\alpha_{k-1} i_k}^{i_{k+1} \dots i_d}, \varepsilon\right)$ ▷ Truncated SVD s. t. $\|\mathtt{tsvd}(A) - A\| \leq \varepsilon$
    $A_k[i_k]_{\alpha_{k-1}}^{\alpha_k} = (U_k)_{\alpha_{k-1} i_k}^{\alpha_k}, \quad \forall\, i_k \in [\![n_k]\!], \alpha_{k-1} \in [\![r_{k-1}]\!], \alpha_k \in [\![r_k]\!]$
    $T_{\alpha_k i_{k+1}}^{i_{k+2} \dots i_d} = \left(\Sigma_k V_k^\mathsf{T}\right)_{\alpha_k}^{i_{k+1} i_{k+2} \dots i_d}, \quad \forall (i_{k+1}, \dots, i_d) \in [\![(n_{k+1}, \dots, n_d)]\!], \alpha_k \in [\![r_k]\!]$
  end for
  $A_d[i_d]^{\alpha_{d-1}} = \left(\Sigma_{d-1} V_{d-1}^\mathsf{T}\right)_{\alpha_{d-1}}^{i_d}, \quad \forall\, i_d \in [\![n_d]\!], \alpha_{d-1} \in [\![r_{d-1}]\!]$
  return $(A_1, \dots, A_d)$
end function

This algorithm [Ose11] is called the HSVD algorithm with truncations or TT-SVD. It is summarised in Algorithm 1.2.

Truncating the successive SVDs gives an estimate on the best approximation by a tensor train of fixed TT ranks.

Theorem 1.2.14 ([Gra10, Ose11, Hac12, Hac14])**.** *Let $\boldsymbol{u} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$, $\tilde{\mathbf{r}} \in \mathbb{N}^{d+1}$ and $\mathscr{M}_{\mathrm{TT} \leq \tilde{\mathbf{r}}}$ be the space of tensor trains of ranks bounded by $\tilde{\mathbf{r}}$. Then we have*

$$\min_{\boldsymbol{v} \in \mathscr{M}_{\mathrm{TT} \leq \tilde{\mathbf{r}}}} \|\boldsymbol{u} - \boldsymbol{v}\| \leq \sqrt{\sum_{k=1}^{d-1} \sum_{\alpha > \tilde{r}_k} {\sigma_\alpha^{(k)}}^2} \leq \sqrt{d-1} \min_{\boldsymbol{v} \in \mathscr{M}_{\mathrm{TT} \leq \tilde{\mathbf{r}}}} \|\boldsymbol{u} - \boldsymbol{v}\|,$$

where for $k \in [\![d-1]\!]$, $(\sigma_\alpha^{(k)})_{\alpha \in [\![r_k]\!]}$ are the singular values of the reshape $(\boldsymbol{u}^{\leq k}) \in \mathbb{R}^{n_1 \cdots n_k \times n_{k+1} \cdots n_d}$.

An important consequence of this theorem is that it is sufficient to derive bounds for the tale of the singular values of each reshape $(\boldsymbol{u}_{i_1 \dots i_k}^{i_{k+1} \dots i_d}) \in \mathbb{R}^{n_1 \cdots n_k \times n_{k+1} \cdots n_d}$ to get bounds on the TT ranks of a TT approximation. This considerably simplifies the question of the approximability by TT of a given tensor, and this characterisation will be used to study the eigenvalue problems of particular operators in Chapter 3.

The proof of this theorem relies on a close inspection of the HSVD algorithm with truncations 1.2. We state a key property of the HSVD algorithm before moving to the proof of the theorem.

Proposition 1.2.15. *For $\varepsilon > 0$, let $(A_k)_{k \in [\![d]\!]}$ be the TT cores obtained from the truncated HSVD algorithm 1.2 for a tensor $\boldsymbol{u} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$ and with tolerance ε. Let $\boldsymbol{u}^\varepsilon$ be the tensor corresponding to the TT cores $(A_k)_{k \in [\![d]\!]}$. Let $\mathrm{id}_{k:d}$ denote the identity on $\mathbb{R}^{n_k \times \cdots \times n_d}$.*

Then there exist a family of orthogonal projectors $(\Pi_k)_{k\in[\![d-1]\!]}$ *with* $\Pi_k \in \mathbb{R}^{n_1\cdots n_k\times n_1\cdots n_k}$ *such that*

$$\boldsymbol{u}^{\varepsilon} = (\Pi_{d-1}\otimes \mathrm{id}_d)(\Pi_{d-2}\otimes \mathrm{id}_{d-1:d})\cdots(\Pi_1\otimes \mathrm{id}_{2:d})\boldsymbol{u} \tag{1.2.5}$$

and for all $k\in[\![d-1]\!]$,

$$\begin{aligned}\Big\|(\Pi_k\otimes \mathrm{id}_{k+1:d})(\Pi_{k-1}\otimes \mathrm{id}_{k:d})\cdots(\Pi_1\otimes \mathrm{id}_{2:d})\boldsymbol{u} - (\Pi_{k-1}\otimes \mathrm{id}_{k:d})\cdots(\Pi_1\otimes \mathrm{id}_{2:d})\boldsymbol{u}\Big\| \\ = \Big(\sum_{\alpha>r_k}\sigma_\alpha\big((\Pi_{k-1}\otimes \mathrm{id}_k)\cdots(\Pi_1\otimes \mathrm{id}_{2:k})\boldsymbol{u}^{\le k}\big)^2\Big)^{1/2},\end{aligned}$$

where $\big(\sigma_\alpha(((\Pi_{k-1}\otimes \mathrm{id}_k)\cdots(\Pi_1\otimes \mathrm{id}_{2:k}))\boldsymbol{u}^{\le k})\big)_\alpha$ *are the singular values of* $(\Pi_{k-1}\otimes \mathrm{id}_k)\cdots(\Pi_1\otimes \mathrm{id}_{2:k})\boldsymbol{u}^{\le k}$.

Proof. For any $k\in[\![d-1]\!]$, let $\boldsymbol{u}^{\varepsilon,k}\in\mathbb{R}^{n_1\times\cdots\times n_d}$ be the tensor obtained at the step k in the truncated HSVD algorithm 1.3

$$(\boldsymbol{u}^{\varepsilon,k})^{\le k} = A_1\bowtie\cdots\bowtie A_k(\Sigma_k V_k^{\mathsf{T}}),$$

where $\bowtie$ is the strong Kronecker product defined in Definition 1.2.10. Let $k\in[\![d-2]\!]$. First note that by definition of A_{k+1}, we have $((A_{k+1}^{\mathsf{T}})^{\le 2})^{\mathsf{T}}(\Sigma_k V_k^{\mathsf{T}})^{i_{k+2}\ldots i_d}_{\alpha_k i_{k+1}} = \Sigma_{k+1}V_{k+1}^{\mathsf{T}}$. Let $\mathscr{A}_k = (A_1\bowtie\cdots\bowtie A_k)^{\le k}$ and $\Pi_{k+1}\in\mathbb{R}^{n_1\cdots n_{k+1}\times n_1\cdots n_{k+1}}$ be defined by $(\Pi_{k+1})^{J_k j_{k+1}}_{I_k i_{k+1}} = (\mathscr{A}_k\bowtie A_{k+1})(\mathscr{A}_k\bowtie A_{k+1})^{\mathsf{T}}_{I_k;i_{k+1};j_{k+1};J_k}$, for all $i_{k+1},j_{k+1}\in[\![n_{k+1}]\!]$ and $I_k,J_k\in\bigtimes_{\ell=1}^{k}[\![n_\ell]\!]$. Since $(A_j)_{j\in[\![k+1]\!]}$ are left-orthogonal, Π_{k+1} is an orthogonal projection. We have

$$\begin{aligned}(\Pi_{k+1}\otimes \mathrm{id}_{k+2:d})\boldsymbol{u}^{\varepsilon,k} &= \big((\mathscr{A}_k\bowtie A_{k+1})(\mathscr{A}_k\bowtie A_{k+1})^{\mathsf{T}}\otimes \mathrm{id}_{k+2:d}\big)(\mathscr{A}_k\bowtie(\Sigma_k V_k^{\mathsf{T}})) \\ &= \big((\mathscr{A}_k\bowtie A_{k+1})\otimes \mathrm{id}_{k+2:d}\big)\big((\mathscr{A}_k\bowtie A_{k+1})^{\mathsf{T}}\otimes \mathrm{id}_{k+2:d}\big)(\mathscr{A}_k\bowtie(\Sigma_k V_k^{\mathsf{T}})) \\ &= \big((\mathscr{A}_k\bowtie A_{k+1})\otimes \mathrm{id}_{k+2:d}\big)\big(((A_{k+1}^{\mathsf{T}})^{\le 2})^{\mathsf{T}}(\Sigma_k V_k^{\mathsf{T}})^{i_{k+2}\ldots i_d}_{\alpha_k i_{k+1}}\big) \\ &= (\mathscr{A}_k\bowtie A_{k+1})\bowtie(\Sigma_{k+1}V_{k+1}^{\mathsf{T}}) = \boldsymbol{u}^{\varepsilon,k+1},\end{aligned}$$

where we have used that $\mathscr{A}_k^{\mathsf{T}}\mathscr{A}_k = \mathrm{id}_{r_k}$. Since $\boldsymbol{u}^{\varepsilon,1} = \Pi_1\otimes \mathrm{id}_{2:d}\,\boldsymbol{u}$, we have by iteration for any $k\in[\![d-1]\!]$

$$\boldsymbol{u}^{\varepsilon,k} = (\Pi_k\otimes \mathrm{id}_{k+1:d})\cdots(\Pi_1\otimes \mathrm{id}_{2:d})\boldsymbol{u}, \tag{1.2.6}$$

and in particular, (1.2.5).

Using notation of the truncated HSVD algorithm 1.2, we have $(A_k^{\le 2},\Sigma_k,V_k^{\mathsf{T}})$ is an SVD of the matrix $\big((\Sigma_{k-1}V_{k-1}^{\mathsf{T}})^{i_{k+1}\ldots i_d}_{\alpha_{k-1}i_k}\big)\in\mathbb{R}^{r_{k-1}n_k\times n_{k+1}\cdots n_d}$ for each $k\in[\![2;d-1]\!]$. Since $\mathscr{A}_{k-1}$ is a partial isometry, we deduce that $((\mathscr{A}_{k-1}\otimes \mathrm{id}_k)A_k^{\le 2},\Sigma_k,V_k^{\mathsf{T}})$ is a truncated SVD of $(\mathscr{A}_{k-1}\otimes \mathrm{id}_k)\big((\Sigma_{k-1}V_{k-1}^{\mathsf{T}})^{i_{k+1}\ldots i_d}_{\alpha_{k-1}i_k}\big)$, which is $(\boldsymbol{u}^{\varepsilon,k-1})^{\le k}$. Now since $(\mathscr{A}_{k-1}\otimes \mathrm{id}_k)A_k^{\le 2} = \mathscr{A}_k$ and $(\boldsymbol{u}^{\varepsilon,k})^{\le k} =$

$\mathscr{A}_k(\Sigma_k V_k^\mathsf{T})$, we have

$$\begin{aligned}\|\boldsymbol{u}^{\varepsilon,k} - \boldsymbol{u}^{\varepsilon,k-1}\| &= \Big\|(\Pi_k \otimes \mathrm{id}_{k+1:d})\cdots(\Pi_1 \otimes \mathrm{id}_{2:d})\boldsymbol{u} - (\Pi_{k-1} \otimes \mathrm{id}_{k:d})\cdots(\Pi_1 \otimes \mathrm{id}_{2:d})\boldsymbol{u}\Big\| \\ &= \Big(\sum_{\alpha>r_k} \sigma_\alpha\big((\Pi_{k-1} \otimes \mathrm{id}_k)\cdots(\Pi_1 \otimes \mathrm{id}_{2:k})\boldsymbol{u}^{\leq k}\big)^2\Big)^{1/2},\end{aligned}$$

where we have used (1.2.6). □

We can now move on to the proof of Theorem 1.2.14.

Proof of Theorem 1.2.14. We begin with the proof of the left-hand side inequality. Using notation from Proposition 1.2.15, we have

$$\begin{aligned}\|\boldsymbol{u}^{\varepsilon} - \boldsymbol{u}\| &= \|(\Pi_{d-1} \otimes \mathrm{id}_d)\cdots(\Pi_1 \otimes \mathrm{id}_{2:d})\boldsymbol{u} - \boldsymbol{u}\| \\ &= \Big\|\sum_{k=1}^{d-1}(\Pi_k \otimes \mathrm{id}_{k+1:d})\cdots(\Pi_1 \otimes \mathrm{id}_{2:d})\boldsymbol{u} - (\Pi_{k-1} \otimes \mathrm{id}_{k:d})\cdots(\Pi_1 \otimes \mathrm{id}_{2:d})\boldsymbol{u}\Big\| \\ &\leq \sum_{k=1}^{d-1}\Big\|(\Pi_k \otimes \mathrm{id}_{k+1:d})\cdots(\Pi_1 \otimes \mathrm{id}_{2:d})\boldsymbol{u} - (\Pi_{k-1} \otimes \mathrm{id}_{k:d})\cdots(\Pi_1 \otimes \mathrm{id}_{2:d})\boldsymbol{u}\Big\| \\ &\leq \sum_{k=1}^{d-1}\Big(\sum_{\alpha>r_k} \sigma_\alpha\big((\Pi_{k-1} \otimes \mathrm{id}_k)\cdots(\Pi_1 \otimes \mathrm{id}_{2:k})\boldsymbol{u}^{\leq k}\big)^2\Big)^{1/2}.\end{aligned}$$

It suffices to prove that for any α_k, we have

$$\sigma_\alpha\big((\Pi_{k-1} \otimes \mathrm{id}_k)\cdots(\Pi_1 \otimes \mathrm{id}_{2:k})\boldsymbol{u}^{\leq k}\big) \leq \sigma_\alpha(\boldsymbol{u}^{\leq k}).$$

As $(\Pi_{k-1} \otimes \mathrm{id}_k)\cdots(\Pi_1 \otimes \mathrm{id}_{2:k})$ is an orthogonal projection, its operator norm is equal to 1. Thus using the variational characterisation of the singular values (1.1.1), we have that

$$\begin{aligned}\sigma_\alpha\big((\Pi_{k-1} \otimes \mathrm{id}_k)\cdots(\Pi_1 \otimes \mathrm{id}_{2:k})\boldsymbol{u}^{\leq k}\big) &\leq \big\|(\Pi_{k-1} \otimes \mathrm{id}_k)\cdots(\Pi_1 \otimes \mathrm{id}_{2:k})\big\|_{\mathrm{op}}\sigma_{\alpha_k}(\boldsymbol{u}^{\leq k}) \\ &\leq \sigma_{\alpha_k}(\boldsymbol{u}^{\leq k}).\end{aligned}$$

This finishes the proof of the left-hand side bound on the best approximation by a tensor train in $\mathscr{M}_{\mathrm{TT}\leq\tilde{\mathbf{r}}}$.

For the lower bound on the best approximation $\boldsymbol{u}_{\mathrm{best}} \in \mathscr{M}_{\mathrm{TT}\leq\tilde{\mathbf{r}}}$, we have for each $k \in [\![d-1]\!]$ by definition of the SVD truncation

$$\|\boldsymbol{u}^{\leq k} - \mathtt{tsvd}(\boldsymbol{u}^{\leq k}, \tilde{r}_k)\|^2 = \sum_{\alpha>\tilde{r}_k} {\sigma_\alpha^{(k)}}^2 \leq \|\boldsymbol{u} - \boldsymbol{u}_{\mathrm{best}}\|^2,$$

as $(\boldsymbol{u}_{\mathrm{best}})_{i_1\ldots i_k}^{i_{k+1}\ldots i_d}$ is a matrix of rank $\tilde{r}_k$. Hence by summing over $k \in [\![d-1]\!]$ we get the lower bound. □

A drawback of the HSVD algorithm or its truncated version is that it requires to handle the full tensor. This means that the cost of the HSVD algorithm with truncations is still exponential in the number of modes d.

If the tensor is already in a TT format, it is possible to reduce the cost of this truncation, provided that the TT cores have the right normalisation. Let $(A_1, \dots, A_d)$ be a right-orthogonal TT representation of the tensor $\boldsymbol{u} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$. The first reshape is

$$\boldsymbol{u}^{\leq 1} = \begin{bmatrix} A_1[1] \\ \vdots \\ A_1[n_1] \end{bmatrix} \begin{bmatrix} A_2[1] \cdots A_d[1] & \dots & A_2[n_2] \cdots A_d[n_d] \end{bmatrix},$$

and since the TT cores $(A_2, \dots, A_d)$ are right-orthogonal, the matrix $V_2 = \begin{bmatrix} A_2[1] \cdots A_d[1] & \dots & A_2[n_2] \cdots A_d[n_d] \end{bmatrix}$ satisfies $V_2 V_2^\mathsf{T} = \mathrm{id}_{r_1}$. Hence the first step of the HSVD truncation can be reduced to the SVD of the reshape of A_1. The same would hold for the next step of the HSVD truncation, hence the total cost of the TT compression of $\boldsymbol{u}$ in a TT format is reduced to $\mathcal{O}(dnr^3)$ where $r = \max(r_k)$ and $n = \max(n_k)$.

The algorithm is summarised in Algorithm 1.3. It is often called *TT rounding* – as it is conceptually the same operation as rounding a float – or *TT compression*.

Algorithm 1.3 TT rounding algorithm

Input: $(A_1, \dots, A_d)$ right-orthogonal TT representation, $\varepsilon > 0$ tolerance
Output: $(A_1^\varepsilon, \dots, A_d^\varepsilon)$ TT representation such that $\|\mathrm{TT}(A_i^\varepsilon) - \mathrm{TT}(A_i)\| \leq \sqrt{d-1}\,\varepsilon$

function TT-ROUNDING($(A_1, \dots, A_d), \varepsilon$)
  for $k = 1, \dots, d-1$ **do**
    $U_k, \Sigma_k, V_k^\mathsf{T} = \mathtt{tsvd}\left(\begin{bmatrix} A_k[1] \\ \vdots \\ A_k[n_k] \end{bmatrix}, \varepsilon \right)$ ▷ Truncated SVD s. t. $\|\mathtt{tsvd}(A) - A\| \leq \varepsilon$
    $r_k = \mathtt{size}(\Sigma_k)$
    $(A_k^\varepsilon)_{i_k \alpha_{k-1}}^{\alpha_k} = (U_k)_{i_k \alpha_{k-1}}^{\alpha_k}, \quad \forall\, i_k \in [\![n_k]\!], \alpha_{k-1} \in [\![r_{k-1}]\!], \alpha_k \in [\![r_k]\!]$
    $A_{k+1}[i_{k+1}] = \Sigma_k V_k^\mathsf{T} A_{k+1}[i_{k+1}], \quad \forall\, i_{k+1} \in [\![n_{k+1}]\!]$ ▷ Root shifting
  end for
  $A_d^\varepsilon = A_d$
  return $(A_1^\varepsilon, \dots, A_d^\varepsilon)$
end function

1.2.5 Gauge fixing

In this section, we give results on the gauge remaining from the TT normalisation introduced in Section 1.2.2. We also present algorithms to obtain a TT decomposition with a prescribed

normalisation.

Such normalisations turn out to be convenient for the computation of the norm a tensor. Suppose that $(A_1, \dots, A_d)$ is a left-orthogonal TT decomposition. The norm of the corresponding tensor $\boldsymbol{u}$ remarkably simplifies

Another instance where the choice of the normalisation is crucial is in solving eigenvalue problems in DMRG (see Chapter 2).

It is also possible to mix both normalisations, in the sense that for some $2 \leq \ell \leq d-1$, we have

In that case, the norm of the tensor is carried by the TT core that is not normalised:

$$\begin{aligned}
\|\boldsymbol{u}\|^2 &= \sum_{i_1=1}^{n_1} \cdots \sum_{i_d=1}^{n_d} A_d[i_d]^\mathsf{T} \cdots A_1[i_1]^\mathsf{T} A_1[i_1] \cdots A_d[i_d] \\
&= \sum_{i_1=1}^{n_1} \cdots \sum_{i_d=1}^{n_d} \operatorname{Tr}\left(A_d[i_d]^\mathsf{T} \cdots A_1[i_1]^\mathsf{T} A_1[i_1] \cdots A_d[i_d]\right) \\
&= \sum_{i_1=1}^{n_1} \cdots \sum_{i_d=1}^{n_d} \operatorname{Tr}\left(A_{\ell+1}[i_{\ell+1}] \cdots A_d[i_d] A_d[i_d]^\mathsf{T} \cdots A_1[i_1]^\mathsf{T} A_1[i_1] \cdots A_\ell[i_\ell]\right) \\
&= \sum_{i_\ell=1}^{n_\ell} \operatorname{Tr}\left(A_\ell[i_\ell]^\mathsf{T} A_\ell[i_\ell]\right).
\end{aligned}$$

A representation of this type can be obtained by slightly modifying the hierarchical SVD described earlier. Instead of performing SVDs from left to right, one stops the SVDs from the left to the cut ℓ and does the SVDs from the right. For example for $\ell = 2$, we have (using again Einstein convention)

$$\begin{aligned}
\boldsymbol{u}_{i_1 \dots i_d} &= \left(\boldsymbol{u}_{i_1}^{i_2 \dots i_d}\right) && \text{(reshape of } \boldsymbol{u} \text{ to } n_1 \times n_2 \cdots n_d) \\
&= \left(U_1\right)_{i_1}^{\alpha_1} \left(\Sigma_1 V_1^\mathsf{T}\right)_{\alpha_1}^{i_2 \dots i_d} && \text{(SVD)} \\
&= \left(U_1\right)_{i_1}^{\alpha_1} \left(\Sigma_1 V_1^\mathsf{T}\right)_{\alpha_1 i_2 \dots i_{d-1}}^{i_d} && \text{(reshape of } \Sigma_1 V_1^\mathsf{T}) \\
&= \left(U_1\right)_{i_1}^{\alpha_1} \left(U_{d-1}\Sigma_{d-1}\right)_{\alpha_1 i_2 \dots i_{d-1}}^{\alpha_{d-1}} \left(V_{d-1}^\mathsf{T}\right)_{\alpha_{d-1}}^{i_d} && \text{(SVD of } \Sigma_1 V_1^\mathsf{T}) \\
&= \left(U_1\right)_{i_1}^{\alpha_1} \left(U_{d-1}\Sigma_{d-1}\right)_{\alpha_1 i_2 \dots i_{d-2}}^{\alpha_{d-1} i_{d-1}} \left(V_{d-1}^\mathsf{T}\right)_{\alpha_{d-1}}^{i_d} && \text{(reshape of } U_{d-1}\Sigma_{d-1}),
\end{aligned}$$

where we repeat the process until we get

$$\boldsymbol{u}_{i_1 \dots i_d} = \left(U_1\right)_{i_1}^{\alpha_1} \left(U_2\Sigma_2\right)_{\alpha_1 i_2}^{\alpha_2} \cdots \left(V_{d-2}^\mathsf{T}\right)_{\alpha_{d-2} i_{d-1}}^{\alpha_{d-1}} \left(V_{d-1}^\mathsf{T}\right)_{\alpha_{d-1}}^{i_d}.$$

The TT decomposition then reads as

$$\begin{aligned}
\boldsymbol{u}_{i_1 \dots i_d} &= \left(U_1\right)_{i_1}^{\alpha_1} \quad \left(U_2\Sigma_2\right)_{\alpha_1 i_2}^{\alpha_2} \quad \cdots \quad \left(V_{d-2}^\mathsf{T}\right)_{\alpha_{d-2} i_{d-1}}^{\alpha_{d-1}} \quad \left(V_{d-1}^\mathsf{T}\right)_{\alpha_{d-1}}^{i_d} \\
&= A_1[i_1]_{\alpha_1} \quad A_2[i_2]_{\alpha_2}^{\alpha_1} \quad \cdots \quad A_{d-1}[i_{d-1}]_{\alpha_{d-1}}^{\alpha_{d-2}} \quad A_d[i_d]^{\alpha_{d-1}},
\end{aligned}$$

where $(A_1, \dots, A_{\ell-1})$ are left-orthogonal and $(A_{\ell+1}, \dots, A_d)$ are right-orthogonal.

Conversion between left and right orthogonal TT representations

By successive LQ decompositions, it is possible to transform a left-orthogonal to a right orthogonal TT decomposition. Let $(A_1, \dots, A_d)$ be a left-orthogonal TT decomposition of $\boldsymbol{u} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$. Then we have

$$\begin{aligned}
\boldsymbol{u}_{i_1 \dots i_d} &= A_1[i_1] \cdots A_d[i_d] \\
&= A_1[i_1]^{\alpha_1} A_2[i_2]^{\alpha_2}_{\alpha_1} \cdots A_{d-1}[i_{d-1}]^{\alpha_{d-1}}_{\alpha_{d-2}} \big(A_d\big)^{i_d}_{\alpha_{d-1}} \\
&= A_1[i_1]^{\alpha_1} A_2[i_2]^{\alpha_2}_{\alpha_1} \cdots A_{d-1}[i_{d-1}]^{\alpha_{d-1}}_{\alpha_{d-2}} \big(L_d\big)^{\beta_{d-1}}_{\alpha_{d-1}} \big(Q_d\big)^{i_d}_{\beta_{d-1}} \\
&= A_1[i_1]^{\alpha_1} A_2[i_2]^{\alpha_2}_{\alpha_1} \cdots A_{d-2}[i_{d-2}]^{\alpha_{d-2}}_{\alpha_{d-3}} \big(A_{d-1}L_d\big)^{i_{d-1}\beta_{d-1}}_{\alpha_{d-2}} \big(Q_d\big)^{i_d}_{\beta_{d-1}} \\
&= A_1[i_1]^{\alpha_1} A_2[i_2]^{\alpha_2}_{\alpha_1} \cdots A_{d-2}[i_{d-2}]^{\alpha_{d-2}}_{\alpha_{d-3}} \big(L_{d-1}\big)^{\beta_{d-2}}_{\alpha_{d-2}} \big(Q_{d-1}\big)^{i_{d-1}\beta_{d-1}}_{\beta_{d-2}} \big(Q_d\big)^{i_d}_{\beta_{d-1}},
\end{aligned}$$

we repeat this process until we reach

$$\begin{aligned}
\boldsymbol{u}_{i_1 \dots i_d} &= \big(A_1 L_2\big)^{i_1 \beta_1} \quad \big(Q_2\big)^{i_2 \beta_2}_{\beta_1} \quad \cdots \quad \big(Q_{d-1}\big)^{i_{d-1}\beta_{d-1}}_{\beta_{d-2}} \quad \big(Q_d\big)^{i_d}_{\beta_{d-1}} \\
&= \quad B_1[i_1]_{\beta_1} \quad B_2[i_2]^{\beta_1}_{\beta_2} \quad \cdots \quad B_{d-1}[i_{d-1}]^{\beta_{d-2}}_{\beta_{d-1}} \quad B_d[i_d]^{\beta_{d-1}}.
\end{aligned}$$

We simply need to check that the TT cores $B_2, \dots, B_d$ are right-orthogonal: for any $k \in [\![2; d]\!]$, we have

$$\sum_{i_k=1}^{n_k} \big(B_k[i_k] B_k[i_k]^\mathsf{T}\big)_{\alpha_{k-1}\tilde{\alpha}_{k-1}} = \sum_{i_k=1}^{n_k} \sum_{\alpha_k=1}^{r_k} (Q_k)^{i_k \alpha_k}_{\alpha_{k-1}} (Q_k)^{i_k \alpha_k}_{\tilde{\alpha}_{k-1}} = \delta_{\alpha_{k-1}\tilde{\alpha}_{k-1}}.$$

These normalisations have the advantage of reducing the gauge freedom in the TT representation.

Proposition 1.2.16 (Gauge freedom of left-orthogonal TT decompositions [HRS12b])**.** *A left-orthogonal TT representation of minimal TT rank $(r_1, \dots, r_{d-1})$ is unique up to the insertion of orthogonal matrices,* i.e. *if $(A_1, \dots, A_d)$ and $(B_1, \dots, B_d)$ are left-orthogonal TT representations of the same tensor $\boldsymbol{u}$, then there are orthogonal matrices $(Q_k)_{1 \le k \le d-1}$, $Q_k \in \mathbb{R}^{r_k \times r_k}$ such that for all $1 \le i_k \le n_k$ we have*

$$\begin{aligned}
A_1[i_1] Q_1 = B_1[i_1], \quad Q_{d-1}^\mathsf{T} A_d[i_d] = B_d[i_d] \\
Q_{k-1}^\mathsf{T} A_k[i_k] Q_k = B_k[i_k], \ \text{for } k = 2, \dots, d-1.
\end{aligned} \tag{1.2.7}$$

Similar statements would be true for other types of normalisations.

Proof. The proof relies on the following observation: let $M_1, N_1 \in \mathbb{R}^{p \times r}$ and $M_2, N_2 \in \mathbb{R}^{r \times q}$ be matrices of rank r such that

$$M_1 M_2 = N_1 N_2 \quad \text{and} \quad M_1^\mathsf{T} M_1 = N_1^\mathsf{T} N_1 = \mathrm{id}_r,$$

there is an orthogonal matrix $Q \in \mathbb{R}^{r\times r}$ such that

$$M_1 = N_1 Q \quad \text{and} \quad M_2 = Q^\mathsf{T} N_2.$$

The proof of this result is straightforward. We have $N_2 = N_1^\mathsf{T} M_1 M_2 = N_1^\mathsf{T} M_1 M_1^\mathsf{T} N_1 N_2$. Since N_2 is full-rank, it shows that $N_1^\mathsf{T} M_1$ is an orthogonal matrix. Denote this matrix Q. Hence $N_2 = Q M_2$ and $M_1 N_1^\mathsf{T} N_1 = M_1$ thus, $N_1 = M_1 Q^\mathsf{T}$.

The proof then goes by iteration. We have

$$\begin{aligned}\big(A_1[i_1]\big)\big(A_2[i_2]\cdots A_d[i_d]\big) &= \big(B_1[i_1]\big)\big(B_2[i_2]\cdots B_d[i_d]\big)\\ \sum_{i_1=1}^{n_1} A_1[i_1]^\mathsf{T} A_1[i_1] &= \sum_{i_1=1}^{n_1} B_1[i_1]^\mathsf{T} B_1[i_1] = \mathrm{id}_{r_1}.\end{aligned}$$

Since $\big(A_1[i_1]\big), \big(A_2[i_2]\cdots A_d[i_d]\big), \big(B_1[i_1]\big)$ and $\big(B_2[i_2]\cdots B_d[i_d]\big)$ have rank r_1, by applying the previous reult, there is an orthogonal matrix $Q_1 \in \mathbb{R}^{r_1\times r_1}$ such that

$$\begin{aligned}A_1[i_1]Q_1 &= B_1[i_1]\\ Q_1^\mathsf{T}\big(A_2[i_2]\cdots A_d[i_d]\big) &= \big(B_2[i_2]\cdots B_d[i_d]\big).\end{aligned}$$

For the next iteration, we have

$$\begin{aligned}\big(Q_1^\mathsf{T} A_2[i_2]\big)\big(A_3[i_3]\cdots A_d[i_d]\big) &= \big(B_2[i_2]\big)\big(B_3[i_3]\cdots B_d[i_d]\big)\\ \sum_{i_2=1}^{n_2} A_2[i_2]^\mathsf{T} Q_1 Q_1^\mathsf{T} A_2[i_2] &= \sum_{i_2=1}^{n_2} B_2[i_2]^\mathsf{T} B_2[i_2] = \mathrm{id}_{r_1}.\end{aligned}$$

Applying again the lemma, we have

$$\begin{aligned}Q_1^\mathsf{T} A_2[i_2] Q_2 &= B_2[i_2]\\ Q_2^\mathsf{T}\big(A_3[i_3]\cdots A_d[i_d]\big) &= \big(B_3[i_3]\cdots B_d[i_d]\big).\end{aligned}$$

By iteration, we prove the proposition. □

The Vidal representation

A convenient - albeit numerically unstable - way to convert easily between left-orthogonal and right-orthogonal TT representations is to use the Vidal representation [Vid03].

Definition 1.2.17 (Vidal representation [Vid03])**.** *Let $\boldsymbol{u} \in \mathbb{R}^{n_1\times\cdots\times n_d}$ be a tensor. We say that $(\Gamma_k)_{1\le k\le d}$, $(\Sigma_k)_{1\le k\le d-1}$ is a Vidal representation if Σ_k are diagonal matrices with positive diagonal entries, for all $\mathbf{i} \in [\![\mathbf{n}]\!]$,*

$$\boldsymbol{u}_{i_1,\dots,i_d} = \Gamma_1[i_1]\Sigma_1\Gamma_2[i_2]\Sigma_2\cdots\Sigma_{d-1}\Gamma_d[i_d], \tag{1.2.8}$$

and for all $k \in [\![d]\!]$, *the matrices* $\Gamma_k \in \mathbb{R}^{n_k \times r_{k-1} \times r_k}$ *satisfy*

$$\sum_{i_1=1}^{n_1} \Gamma_1[i_1]^\mathsf{T} \Gamma_1[i_1] = \mathrm{id}_{r_1}, \quad \sum_{i_d=1}^{n_d} \Gamma_d[i_d] \Gamma_d[i_d]^\mathsf{T} = \mathrm{id}_{r_{d-1}} \tag{1.2.9}$$

$$\forall\, k = 2, \dots, d-1, \ \sum_{i_k=1}^{n_k} \Gamma_k[i_k]^\mathsf{T} \Sigma_{k-1}^2 \Gamma_k[i_k] = \mathrm{id}_{r_k}, \quad \sum_{i_k=1}^{n_k} \Gamma_k[i_k] \Sigma_k^2 \Gamma_k[i_k]^\mathsf{T} = \mathrm{id}_{r_{k-1}}\,. \tag{1.2.10}$$

The Vidal representation directly gives left and right orthogonal TT decompositions:

(i). $(A_1, \dots, A_d)$ left-orthogonal TT representation

$$\begin{aligned} A_1[i_1] &= \Gamma_1[i_1], \quad A_d[i_d] = \Sigma_{d-1} \Gamma_d[i_d] \\ A_k[i_k] &= \Sigma_{k-1} \Gamma_k[i_k], \quad k \in [\![2; d-1]\!]; \end{aligned}$$

(ii). $(B_1, \dots, B_d)$ right-orthogonal TT representation

$$\begin{aligned} B_1[i_1] &= \Gamma_1[i_1] \Sigma_1, \quad B_d[i_d] = \Gamma_d[i_d] \\ B_k[i_k] &= \Gamma_k[i_k] \Sigma_k, \quad k \in [\![2; d-1]\!]. \end{aligned}$$

The conversion from left (or right) orthogonal decomposition to a Vidal representation is more involved [Sch11, Section 4.6]. Let $(A_k)_{1 \le k \le d}$ be the TT components of a left-orthogonal TT representation. Then we have

$$\boldsymbol{u}_{i_1 \dots i_k}^{i_{k+1} \dots i_d} = \underbrace{\begin{bmatrix} A_1[1] A_2[1] \cdots A_k[1] \\ \vdots \\ A_1[n_1] A_2[n_2] \cdots A_k[n_k] \end{bmatrix}}_{=: M_k \in \mathbb{R}^{n_1 \cdots n_k \times r_k}} \underbrace{\begin{bmatrix} A_{k+1}[i_{k+1}] & \cdots & A_d[i_d] \end{bmatrix}}_{\in \mathbb{R}^{r_k \times n_{k+1} \cdots n_d}}$$

Because (A_k) are left-orthogonal, then for all $k \in [\![d-1]\!]$, $M_k^\mathsf{T} M_k = \mathrm{id}_{r_k}$, hence the singular values of the reshaped tensor are exactly the singular values of the right matrix.

With this remark, we can now write the iterative algorithm to get the Vidal representation of the tensor.

Algorithm 1.4 Left-orthogonal to Vidal representation

Input: $(A_1, \dots, A_d)$ left-orthogonal TT representation
Output: $(\Gamma_1, \dots, \Gamma_d), (\Sigma_1, \dots, \Sigma_{d-1})$ Vidal representation

function LEFTTOVIDAL($(A_1, ..., A_d)$)
  $U_{d-1}, \Sigma_{d-1}, V_d^\intercal = \texttt{svd}\big(\begin{bmatrix} A_d[1] & A_d[2] & \cdots & A_d[n_d] \end{bmatrix} \big)$
  $\begin{bmatrix} \Gamma_d[1] & \cdots & \Gamma_d[n_d] \end{bmatrix} = V_d^\intercal$
  for $k = d-1, \dots, 1$ **do**
    $U_{k-1}, \Sigma_{k-1}, V_k^\intercal = \texttt{svd}\big(\begin{bmatrix} A_k[1]U_k\Sigma_k & \cdots & A_k[n_k]U_k\Sigma_k \end{bmatrix} \big)$.
    Γ_k solution to $V_k^\intercal = \begin{bmatrix} \Gamma_k[1]\Sigma_k & \cdots & \Gamma_k[n_k]\Sigma_k \end{bmatrix}$
  end for
  return $(\Gamma_1, \dots, \Gamma_d), (\Sigma_1, \dots, \Sigma_{d-1})$.
end function

By induction, one can show that the singular values of the successive SVD in the previous algorithm are indeed the singular values of the tensor reshape.

Proposition 1.2.18. *Let $(\Gamma_k)_{1\le k\le d}$, $(\Sigma_k)_{1\le k\le d-1}$ be a Vidal representation of $\boldsymbol{u} \in \mathbb{R}^{n_1\times\cdots\times n_d}$. Then Σ_k is the matrix of the singular values of the reshape $\boldsymbol{u}_{i_1\dots i_k}^{i_{k+1}\dots i_d} \in \mathbb{R}^{n_1\cdots n_k \times n_{k+1}\cdots n_d}$.*

Proof. By definition of the SVD, the Vidal TT components Γ_k satisfy

$$\sum_{i_k=1}^{n_k} \Gamma_k[i_k]\Sigma_k^2\Gamma_k[i_k]^\intercal = \mathrm{id}_{r_{k-1}} .$$

We also have

$$\begin{bmatrix} A_k[1]U_k & \cdots A_k[n_k]U_k \end{bmatrix} = \begin{bmatrix} U_{k-1}\Sigma_{k-1}\Gamma_k[1] & \cdots & U_{k-1}\Sigma_{k-1}\Gamma_k[n_k] \end{bmatrix} .$$

Thus

$$\begin{aligned} \sum_{i_k}^{n_k} \Gamma_k[i_k]^\intercal\Sigma_{k-1}^2\Gamma_k[i_k] &= \sum_{i_k}^{n_k} \Gamma_k[i_k]^\intercal\Sigma_{k-1}U_{k-1}^\intercal U_{k-1}\Sigma_{k-1}\Gamma_k[i_k] \\ &= \sum_{i_k}^{n_k} U_k^\intercal A_k[i_k]^\intercal A_k[i_k]U_k \\ &= \mathrm{id}_{r_k} . \end{aligned}$$

□

1.3 Manifold of tensor trains

Proposition 1.3.1. *The set of tensor trains with TT rank* $\mathbf{r} = (r_1, \dots, r_{d-1})$

$$\mathscr{M}_{\mathrm{TT}_\mathbf{r}} = \Big\{ \boldsymbol{u} \mid \ \exists (A_k)_{k\in[\![d]\!]} \in \bigtimes_{k\in[\![d]\!]} \mathbb{R}^{n_k \times r_{k-1} \times r_k},\ \forall\, \mathbf{i} \in [\![\mathbf{n}]\!], \boldsymbol{u}_{i_1 \dots i_d} = A_1[i_1] \cdots A_d[i_d], \\ \forall\, k \in [\![d-1]\!],\ \mathrm{rank}(\boldsymbol{u}^{i_{k+1}\dots i_d}_{i_1 \dots i_k}) = r_k \Big\},$$

is a manifold of dimension

$$\dim \mathscr{M}_{\mathrm{TT}_\mathbf{r}} = \sum_{i=1}^{d} r_{i-1} n_i r_i - \sum_{i=1}^{d-1} r_i^2. \tag{1.3.1}$$

Proof. Two TT representations $(A_1, \dots, A_d)$ and $(\tilde{A}_1, \dots, \tilde{A}_d)$ of a same tensor are related by a gauge $(G_1, \dots, G_{d-1}) \in \mathrm{GL}_{r_1}(\mathbb{R}) \times \cdots \mathrm{GL}_{r_{d-1}}(\mathbb{R})$

$$\forall\, 1 \le i_k \le n_k, A_k[i_k] = G_{k-1} \tilde{A}_k[i_k] G_k, \quad k = 1, \dots, d, \quad (G_0 = G_d = 1).$$

The dimension of $\mathrm{GL}_{r_k}(\mathbb{R})$ is r_k^2, hence the dimension of $\mathscr{M}_{\mathrm{TT}_\mathbf{r}}$ is

$$\dim \mathscr{M}_{\mathrm{TT}_\mathbf{r}} = \sum_{i=1}^{d} r_{i-1} n_i r_i - \sum_{i=1}^{d-1} r_i^2.$$

□

Proposition 1.3.2 (Tangent space of $\mathscr{M}_{\mathrm{TT}_\mathbf{r}}$ [HRS12b])**.** *Let* $A \in \mathscr{M}_{\mathrm{TT}_\mathbf{r}}$ *and* $(A_1, \dots, A_d)$ *be a left-orthogonal TT representation of* A*. Let* $\delta A \in \mathcal{T}_A \mathscr{M}_{\mathrm{TT}_\mathbf{r}}$*.*

There are unique components $(W_k)_{1\le k\le d} \in \bigotimes_{k=1}^{d} \mathbb{R}^{r_{k-1} \times n_k \times r_k}$ *such that*

$$\delta A = \sum_{k=1}^{d} \delta A^{(k)}, \tag{1.3.2}$$

with

$$\delta A^{(k)}_{i_1 \dots i_d} = A_1[i_1] \cdots A_{k-1}[i_{k-1}] W_k[i_k] A_{k+1}[i_{k+1}] \cdots A_d[i_d], \tag{1.3.3}$$

and where for $k \in [\![d-1]\!]$ *we have*

$$\sum_{i_k=1}^{n_k} A_k[i_k]^{\mathsf{T}} W_k[i_k] = \mathbf{0}_{r_k \times r_k}. \tag{1.3.4}$$

Proof. By definition of the tangent space $\mathcal{T}_A\mathscr{M}_{\mathrm{TT}_\mathbf{r}}$, the tangent vectors are given by the derivatives $\dot{\Gamma}$ of the differentiable curves $\Gamma : \mathbb{R} \to \mathscr{M}_{\mathrm{TT}_\mathbf{r}}$ such that $\Gamma(0) = A$.

For all $t \in \mathbb{R}$, since $\Gamma(t) \in \mathscr{M}_{\mathrm{TT}_\mathbf{r}}$, we can choose a left-orthogonal TT representation of $\Gamma(t)$ such that

$$\Gamma(t)_{i_1 \dots i_d} = \Gamma_1^{(t)}[i_1] \cdots \Gamma_d^{(t)}[i_d],$$

where for all $1 \leq k \leq d$, $t \mapsto \Gamma_k^{(t)} \in \mathbb{R}^{n_k \times r_{k-1} \times r_k}$ is differentiable and $\Gamma_k^{(0)} = A_k$.

Since for $k \in [\![d-1]\!]$, $\sum_{i_k=1}^{n_k} \Gamma_k^{(t)}[i_k]^\mathsf{T} \Gamma_k^{(t)}[i_k] = \mathrm{id}_{r_k}$, there is a differentiable function $t \mapsto U_k(t) \in \mathcal{O}_{n_k r_{k-1}}(\mathbb{R})$ such that

$$\begin{bmatrix} \Gamma_k^{(t)}[1] \\ \vdots \\ \Gamma_k^{(t)}[n_k] \end{bmatrix} = U_k(t) \begin{bmatrix} A_k[1] \\ \vdots \\ A_k[n_k] \end{bmatrix}.$$

This implies that $\begin{bmatrix} \dot{\Gamma}_k^{(0)}[1] \\ \vdots \\ \dot{\Gamma}_k^{(0)}[n_k] \end{bmatrix} = S_k \begin{bmatrix} A_k[1] \\ \vdots \\ A_k[n_k] \end{bmatrix}$ for some antisymmetric matrix $S_k \in \mathbb{R}^{n_k r_{k-1} \times n_k r_{k-1}}$.

Let

$$\begin{bmatrix} W_k[1] \\ \vdots \\ W_k[n_k] \end{bmatrix} = S_k \begin{bmatrix} A_k[1] \\ \vdots \\ A_k[n_k] \end{bmatrix}.$$

Then

$$\sum_{i_k=1}^{n_k} A_k[i_k]^\mathsf{T} W_k[i_k] = \begin{bmatrix} A_k[1]^\mathsf{T} & \dots & A_k[n_k]^\mathsf{T} \end{bmatrix} S_k \begin{bmatrix} A_k[1] \\ \vdots \\ A_k[n_k] \end{bmatrix},$$

which is a symmetric and an antisymmetric matrix, hence it is zero.

The tangent vectors are hence necessarily of the form given by eq. (1.3.2)-(1.3.4). Dimension counting and invoking Proposition 1.3.1 show the uniqueness of the representation. □

Chapter 2

The DMRG algorithm

Density matrix renormalisation group [Whi92] (DMRG) is an alternating scheme to solve linear problems or eigenvalue problems in the tensor train format. In the mathematical community, it is also referred to the *alternating linear scheme* (ALS) in its simplest version or to the *modified ALS (MALS)* [HRS12a], which is the equivalent to the two-site DMRG. In DMRG, given a symmetric matrix $\boldsymbol{\mathcal{H}} \in \mathbb{R}^{n_1 \cdots n_d \times n_1 \cdots n_d}$, we want to solve for $\boldsymbol{x}_* \in \mathbb{R}^{n_1 \cdots n_d}$ the linear problem

$$\boldsymbol{\mathcal{H}} \boldsymbol{x}_* = \boldsymbol{b}, \tag{2.0.1}$$

for a given $\boldsymbol{b} \in \mathbb{R}^{n_1 \cdots n_d}$, or for $(\lambda, \boldsymbol{x}_*) \in \mathbb{R} \times \left(\mathbb{R}^{n_1 \cdots n_d} \setminus \{0\}\right)$ the lowest eigenvalue problem

$$\boldsymbol{\mathcal{H}} \boldsymbol{x}_* = \lambda \boldsymbol{x}_*, \tag{2.0.2}$$

For both problems, a tensor train representation of the operator $\boldsymbol{\mathcal{H}}$ is needed in order to efficiently implement the DMRG algorithm.

2.1 Tensor train operators

2.1.1 Graphical representation of tensors

As we are going to manipulate formulas involving more and more tensors, it can be helpful to have graphical representations of the summation over shared indices between tensors. This operation is called *tensor contraction*.

Let $\boldsymbol{u} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$ be a tensor. The graphical representation of $\boldsymbol{u}$ is given by Figure 2.1. Elementary operations between vectors and matrices are explained in Figure 2.2.

2.1.2 Definition of tensor train operators

Definition 2.1.1 (Tensor train operator)**.** *Let $\boldsymbol{\mathcal{H}} \in \mathbb{R}^{n_1 \cdots n_d \times n_1 \cdots n_d}$ be a matrix. A tensor train operator (TTO) representation of the matrix is any tuple of order 4 tensors $(H_1, \ldots, H_d)$,*

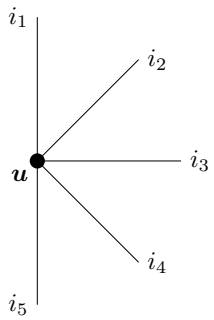
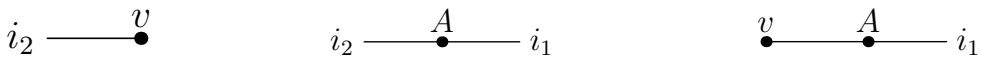


Figure 2.1: Graphical representation of an order 5 tensor $\boldsymbol{u}$. The tensor $\boldsymbol{u}$ is represented by its vertex and its indices by the five free edges.



(a) Vector v_{i_2}. (b) Matrix $A^{i_2}_{i_1}$. (c) Matrix-vector product $(Av)_{i_1} = \sum_{i_2} A^{i_2}_{i_1} v_{i_2}$.

Figure 2.2: Contraction of tensors. Every pair of connected edges is a summation over the shared index.

$H_k \in \mathbb{R}^{R_{k-1} \times n_k \times n_k \times R_k}$ *($R_0 = R_d = 1$) such that*

$$\forall \mathbf{i}, \mathbf{j} \in [\![\mathbf{n}]\!], \boldsymbol{\mathcal{H}}^{j_1 \dots j_d}_{i_1 \dots i_d} = H_1[i_1, j_1] \cdots H_d[i_d, j_d],$$

or written with the strong Kronecker product

$$\boldsymbol{\mathcal{H}} = H_1 \bowtie \cdots \bowtie H_d.$$

$(R_0, \dots, R_d)$ are the TTO ranks of the TTO representation $(H_1, \dots, H_d)$. $(H_1, \dots, H_d)$ are the TTO cores of the TTO representation.

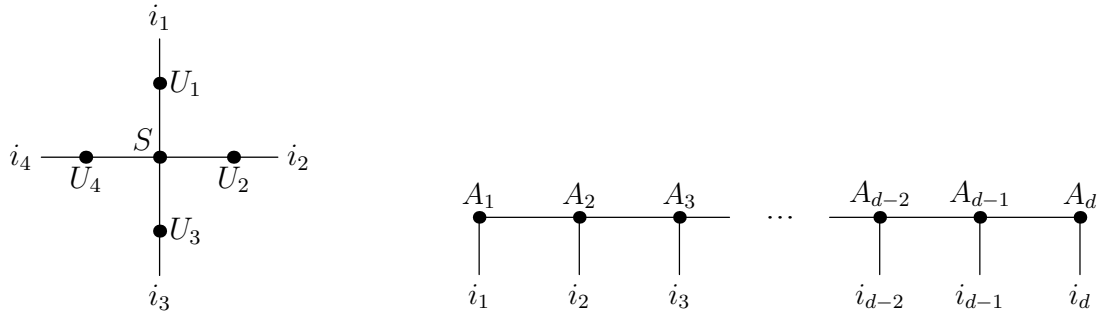
In the context of tensor trains, this is the natural generalisation of the tensor product of operators. Indeed let $h_k \in \mathbb{R}^{n_k \times n_k}$ for $k \in [\![d]\!]$, then the operator $\boldsymbol{\mathcal{H}} = h_1 \otimes \cdots \otimes h_d$ has a TTO representation of TTO rank 1 with TTO cores given by $H_k[i_k, j_k] = (h_k)_{i_k, j_k}$ for $k \in [\![d]\!]$.

The diagrammatic representation of a TTO is similar to the diagrammatic of a TT as illustrated in Figure 2.4.

A TTO representation of a matrix can be obtained by reordering the indices of the matrix $\boldsymbol{\mathcal{H}}$ and performing a TT-SVD on the resulting tensor. More precisely, by defining the tensor $\widetilde{\boldsymbol{\mathcal{H}}} \in \mathbb{R}^{n_1^2 \times \cdots \times n_d^2}$

$$\widetilde{\boldsymbol{\mathcal{H}}}_{i_1 j_1; \dots; i_d j_d} = \boldsymbol{\mathcal{H}}^{j_1 \dots j_d}_{i_1 \dots i_d},$$

we realise that a TTO representation is simply a TT representation of $\widetilde{\boldsymbol{\mathcal{H}}}$.



(a) Tucker decomposition (b) Tensor train decomposition

Figure 2.3: Tucker and tensor train decompositions. From the graphical representation, at first sight we see that the Tucker format still has an exponential dependence in the order of the tensor, whereas this exponential dependence has disappeared in the TT format.

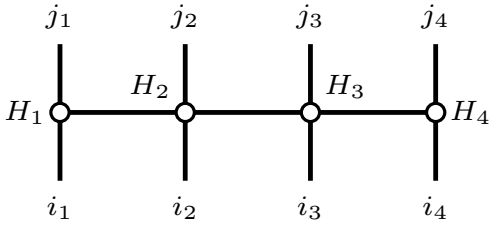


Figure 2.4: Diagrammatic representation of a TTO

2.1.3 Algebraic properties

Like the TT representation of vectors, the TTO format has some algebraic stability property.

Proposition 2.1.2. *Let $\boldsymbol{\mathcal{G}}, \boldsymbol{\mathcal{H}} \in \mathbb{R}^{n_1 \cdots n_d \times n_1 \cdots n_d}$ be matrices and $(G_1, \ldots, G_d)$, $G_k \in \mathbb{R}^{R^G_{k-1} \times n_k \times n_k \times R^G_k}$ and $(H_1, \ldots, H_d)$, $H_k \in \mathbb{R}^{R^H_{k-1} \times n_k \times n_k \times R^H_k}$ be respectively TTO representations of $\boldsymbol{\mathcal{G}}$ and $\boldsymbol{\mathcal{H}}$. Let $\boldsymbol{x} \in \mathbb{R}^{n_1 \cdots n_d}$ be vectors with respective TT representations $(X_1, \ldots, X_d)$, $X_k \in \mathbb{R}^{n_k \times r^A_{k-1} \times r^A_k}$. Then*

(i). the sum $\boldsymbol{\mathcal{G}} + \boldsymbol{\mathcal{H}}$ has a TTO representation $(S_1, \ldots, S_d)$ given by

$$\begin{aligned} S_1[i_1, j_1] &= \begin{bmatrix} G_1[i_1, j_1] & H_1[i_1, j_1] \end{bmatrix}, \quad S_d[i_d, j_d] = \begin{bmatrix} G_d[i_d, j_d] \\ H_d[i_d, j_d] \end{bmatrix} \\ S_k[i_k, j_k] &= \begin{bmatrix} G_k[i_k, j_k] & 0 \\ 0 & H_k[i_k, j_k] \end{bmatrix}, k = 2, \ldots, d-1 \end{aligned} \tag{2.1.1}$$

(ii). the matrix-vector product $\boldsymbol{y} = \boldsymbol{\mathcal{H}}\boldsymbol{x}$ has a TT representation $(Y_1, \ldots, Y_d)$ with $Y_k[j_k] \in$

$\mathbb{R}^{R^H_{k-1} r^X_{k-1} \times R^H_k r^X_k}$

$$Y_k[i_k] = \sum_{j_k=1}^{n_k} H_k[i_k, j_k] \otimes X_k[j_k], \quad k \in [\![d]\!]. \tag{2.1.2}$$

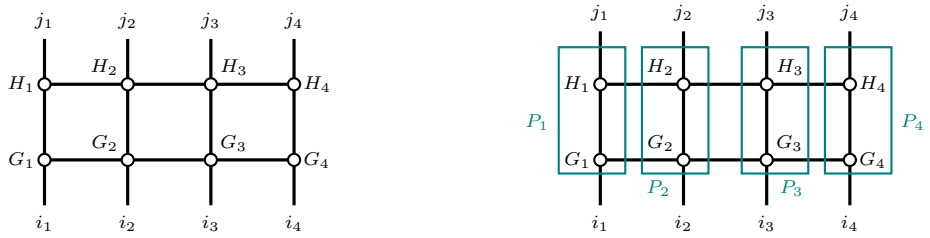
(iii). the product $\boldsymbol{\mathcal{G}}\boldsymbol{\mathcal{H}}$ has a TTO representation $(P_1, \dots, P_d)$ given by

$$P_k[i_k, j_k] = \sum_{\ell_k=1}^{n_k} G_k[i_k, \ell_k] \otimes H_k[\ell_k, j_k], \quad k \in [\![d]\!]. \tag{2.1.3}$$

Proof. This is a direct computation. □

Remark 2.1.3. *The TTO representations of the sum and the product of the operators are not optimal. This is clear in the case of the sum $\boldsymbol{\mathcal{G}} + \boldsymbol{\mathcal{H}}$ when we consider $\boldsymbol{\mathcal{G}} = \boldsymbol{\mathcal{H}}$. A TT rounding step is required in order to reduce the TTO ranks of the representation. This is not innocuous as essential properties of the matrix can be lost in the rounding procedure (symmetry for instance).*

A diagrammatic proof of the formula for the product of two TTO representations is given in Figure 2.5, avoiding cumbersome computations.



(a) Diagrammatic representation of the product of two TTO

(b) Diagrammatic representation of the product of two TTO

Figure 2.5: Diagrammatic proof of the product of two TTO. The left panel is the diagrammatic representation of the product of two TTO. On the right panel, the boxed tensors P_k are the TTO cores of a TTO representation of the product GH, provided that the double edges shared between neighbouring P_k are gathered into one edge.

Example 2.1.4. *Let us consider the following matrix $\boldsymbol{\mathcal{H}} \in \mathbb{R}^{n^d \times n^d}$*

$$\boldsymbol{\mathcal{H}} = h \otimes \mathrm{id} \otimes \cdots \otimes \mathrm{id} + \cdots + \mathrm{id} \otimes \mathrm{id} \otimes \cdots \otimes h,$$

where $h \in \mathbb{R}^{n \times n}$ is a symmetric matrix and id *is the identity in $\mathbb{R}^{n \times n}$. Since the matrix $h \otimes \mathrm{id} \otimes \cdots \otimes \mathrm{id}$ is a TTO of rank 1, a naïve application of Proposition 2.1.2 yields a TTO*

representation of $\boldsymbol{\mathcal{H}}$ of rank d. However it is possible to achieve a rank 2 representation with the following construction

$$\begin{aligned} H_1[i_1, j_1] &= \begin{bmatrix} h_{i_1 j_1} & \delta_{i_1 j_1} \end{bmatrix}, \quad H_d[i_d, j_d] = \begin{bmatrix} \delta_{i_d j_d} \\ h_{i_d j_d} \end{bmatrix} \\ H_k[i_k, j_k] &= \begin{bmatrix} \delta_{i_k j_k} & 0 \\ h_{i_k j_k} & \delta_{i_k j_k} \end{bmatrix}, \quad k = 2, \dots, d-1. \end{aligned} \tag{2.1.4}$$

Note that this representation also satisfies the property stated in Proposition 2.1.5.

Proposition 2.1.5. *Let $\boldsymbol{\mathcal{H}} \in \mathbb{R}^{n_1 \cdots n_d \times n_1 \cdots n_d}$ be a symmetric matrix. Then there is a TTO representation of $\boldsymbol{\mathcal{H}}$ such that*

$$\forall\, 1 \leq i_k, j_k \leq n_k, \;\; H_k[i_k, j_k] = H_k[j_k, i_k], \quad k = 1, \dots, L. \tag{2.1.5}$$

Proof. □

2.1.4 The electronic Hamiltonian as a TTO

The electronic Hamiltonian operator in second quantisation is given by

$$\boldsymbol{\mathcal{H}} = \sum_{i,j=1}^{d} h_{ij} c_i^\dagger c_j + \frac{1}{2} \sum_{i,j,k,\ell=1}^{d} V_{ijk\ell} c_i^\dagger c_j^\dagger c_\ell c_k, \tag{2.1.6}$$

where h_{ij} (resp. $V_{ijk\ell}$) correspond to the one-electron integrals and two-electron integrals with Mulliken's convention [HJO14]. The tensor representation of the creation $c_i^\dagger$ and annihilation c_i operators can be written as a tensor product of 2×2 matrices

$$c_i = Z \otimes \cdots \otimes Z \otimes C \otimes \mathrm{id}_2 \otimes \cdots \otimes \mathrm{id}_2 \in \mathbb{R}^{2^d \times 2^d}, \tag{2.1.7}$$

$$c_i^\dagger = Z \otimes \cdots \otimes Z \otimes C^\mathsf{T} \otimes \mathrm{id}_2 \otimes \cdots \otimes \mathrm{id}_2 \in \mathbb{R}^{2^d \times 2^d}, \tag{2.1.8}$$

where C (resp. C^T) appears in the i-th position and

$$C = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad \text{and} \quad Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

Since the creation and annihilation operators are written as Kronecker products, their TTO rank is 1. Using the algebraic properties of TTOs in Proposition 2.1.2, a naïve implementation of the TTO of an electronic Hamiltonian has TTO rank scaling as d^4.

Noticing that the reshape of the two-body interaction at any cut is at most of rank d^2, we deduce that the TTO rank of the electronic Hamiltonian can be reduced to $\mathcal{O}(d^2)$ [CKN+16, BGP22]. The TT-SVD is useful to compress these ranks to the optimal ones. To preserve the particle conservation and the symmetry of the Hamiltonian, this procedure has to done with great care.

Remark 2.1.6. *In popular implementations of QC-DMRG, it is usual to work in the* space orbital picture. *Namely instead of having sites that can be either occupied or unoccupied, sites can be unoccupied, occupied with spin up or down, or doubly occupied. The expression of the electronic Hamiltonian is similar to the spin orbital case. The main reason of using this representation is that it is more suited for an implementation that preserves the $SU(2)$ symmetry.*

2.2 The DMRG algorithm

The DMRG algorithm [Whi92] is an algorithm to solve linear systems $\boldsymbol{\mathcal{H}}\boldsymbol{x}_* = \boldsymbol{b}$ or the lowest eigenvalue problem $\boldsymbol{\mathcal{H}}\boldsymbol{x}_* = \lambda\boldsymbol{x}_*$ using the variational characterisation of the solution to both problems. As such it is limited in the resolution of linear problems with *symmetric* and positive-definite matrices. In the following, we assume that $\boldsymbol{\mathcal{H}}$ is a symmetric, positive-definite matrix.

Assumption 2.2.1. *The matrix $\boldsymbol{\mathcal{H}} \in \mathbb{R}^{n_1\cdots n_d \times n_1 \cdots n_d}$ is symmetric and positive-definite.*

The solution to the linear system $\boldsymbol{\mathcal{H}}\boldsymbol{x}_* = \boldsymbol{b}$ is also the minimiser of the functional

$$\boldsymbol{x}_* = \underset{\boldsymbol{x}\in\mathbb{R}^{n_1\cdots n_d}}{\arg\min} \frac{1}{2}\langle \boldsymbol{x}, \boldsymbol{\mathcal{H}}\boldsymbol{x}\rangle - \langle \boldsymbol{b}, \boldsymbol{x}\rangle. \tag{2.2.1}$$

Using the Rayleigh-Ritz principle, the lowest eigenvalue of $\boldsymbol{\mathcal{H}}$ is given by

$$\boldsymbol{x}_* = \underset{x\in\mathbb{R}^{n_1\cdots n_d}}{\arg\min} \frac{\langle \boldsymbol{x}, \boldsymbol{\mathcal{H}}\boldsymbol{x}\rangle}{\langle \boldsymbol{x}, \boldsymbol{x}\rangle}. \tag{2.2.2}$$

The first idea in DMRG is to reduce the minimisation set to the set of TT tensors with prescribed TT ranks $\mathbf{r}$

$$\mathscr{M}_{\mathrm{TT}_{\leq \mathbf{r}}} = \left\{ \boldsymbol{u} \mid \exists (A_k)_{k\in[\![d]\!]} \in \bigtimes_{k\in[\![d]\!]} \mathbb{R}^{n_k \times r_{k-1}\times r_k},\ \forall \mathbf{i} \in [\![\mathbf{n}]\!],\ \boldsymbol{u}_{i_1\ldots i_d} = A_1[i_1]\cdots A_d[i_d] \right\},$$

and thus solve, for example in the linear solve case, the following problem

$$\boldsymbol{x}_* = \underset{\boldsymbol{x}\in\mathscr{M}_{\mathrm{TT}_{\leq \mathbf{r}}}}{\arg\min} \frac{1}{2}\langle \boldsymbol{x}, \boldsymbol{\mathcal{H}}\boldsymbol{x}\rangle - \langle \boldsymbol{b}, \boldsymbol{x}\rangle. \tag{2.2.3}$$

The practical trump of the DMRG algorithm now relies on the fact that the approximate minimisation problem above is solved by a sequence of much smaller symmetric positive-definite linear systems of size $\mathcal{O}(r_{\mathrm{TT}}^2 R_{\mathrm{TTO}})$. These problems are tractable and moreover it is possible to import all the technology developed in numerical linear algebra to solve these problems efficiently.

2.2.1 General algorithm

The DMRG algorithm, also known as *alternating linear scheme* (ALS) [HRS12a], is an alternating optimisation over the set $\mathscr{M}_{\mathrm{TT}_{\leq \mathbf{r}}}$. The general idea is to perform a descent step for each TT core separately. Let TT be the map

$$\mathrm{TT} : \begin{cases} \mathbb{R}^{r_0 \times n_1 \times r_1} \times \cdots \times \mathbb{R}^{r_{d-1} \times n_d \times r_d} \to \mathbb{R}^{n_1 \cdots n_d} \\ \qquad (X_1, \ldots, X_d) \mapsto X_1 \bowtie \cdots \bowtie X_d = (X_1[i_1] \cdots X_d[i_d]), \end{cases}$$

Introducing the functional $J(\boldsymbol{x}) = \frac{1}{2}\langle \boldsymbol{x}, \boldsymbol{\mathcal{H}}\boldsymbol{x}\rangle - \langle \boldsymbol{b}, \boldsymbol{x}\rangle$ and j the map

$$j(X_1, \ldots, X_d) = J \circ \mathrm{TT}(X_1, \ldots, X_d), \tag{2.2.4}$$

then minimising J over the manifold $\mathscr{M}_{\mathrm{TT}_{\leq \mathbf{r}}}$ is the same as minimising the functional j over the product space $\mathbb{R}^{n_1 \times r_1} \times \mathbb{R}^{r_1 \times n_2 \times r_2} \times \cdots \times \mathbb{R}^{r_{d-1} \times n_d}$:

$$\min_{\boldsymbol{x} \in \mathscr{M}_{\mathrm{TT}_{\leq \mathbf{r}}}} \frac{1}{2}\langle \boldsymbol{x}, \boldsymbol{\mathcal{H}}\boldsymbol{x}\rangle - \langle \boldsymbol{b}, \boldsymbol{x}\rangle = \min_{X_1, \ldots, X_d} j(X_1, \ldots, X_d).$$

In the one-site DMRG procedure, the minimisation of j is carried out sequentially over (X_k) by freezing all the TT cores but one and by solving the minimisation problem for the remaining core. More precisely, for $k \in [\![d]\!]$, let P_k be defined by

$$P_k : \begin{cases} \mathbb{R}^{r_{k-1} \times n_k \times r_k} \to \mathbb{R}^{n_1 \times \cdots \times n_d} \\ \qquad V \mapsto X_1 \bowtie \cdots \bowtie X_{k-1} \bowtie V \bowtie X_{k+1} \bowtie \cdots X_d. \end{cases} \tag{2.2.5}$$

The minimisation problem to solve is the following

$$\min_{V \in \mathbb{R}^{r_{k-1} \times n_k \times r_k}} J(P_k V) = \min_{V \in \mathbb{R}^{r_{k-1} \times n_k \times r_k}} \frac{1}{2}\langle P_k V, \boldsymbol{\mathcal{H}} P_k V\rangle - \langle \boldsymbol{b}, P_k V\rangle.$$

If the minimiser is denoted by Y_k, it thus solves

$$P_k^{\mathsf{T}} \boldsymbol{\mathcal{H}} P_k Y_k = P_k^{\mathsf{T}} \boldsymbol{b}. \tag{2.2.6}$$

A natural condition to impose on P_k is that it is a partial isometry, for the following reason.

Proposition 2.2.2. *If P_k is a partial isometry, then the linear system (2.2.6) has a unique solution.*

Moreover the condition number of the linear system (2.2.6) is bounded by the condition number of $\boldsymbol{\mathcal{H}}$, i.e.

$$\mathrm{cond}_2 P_k^{\mathsf{T}} \boldsymbol{\mathcal{H}} P_k \leq \mathrm{cond}_2 \boldsymbol{\mathcal{H}}.$$

Proof. Since P_k is a partial isometry, the matrix $P_k^\mathsf{T} \boldsymbol{\mathcal{H}} P_k$ is symmetric positive-definite, thus the linear system has a unique solution.

The bound on the condition number follows from the fact that P_k is a partial isometry, as we have the inequalities $\lambda_{\min}(P_k^\mathsf{T} \boldsymbol{\mathcal{H}} P_k) \geq \lambda_{\min}(\boldsymbol{\mathcal{H}})$ and $\lambda_{\max}(P_k^\mathsf{T} \boldsymbol{\mathcal{H}} P_k) \leq \lambda_{\max}(\boldsymbol{\mathcal{H}})$. □

It is rather simple to impose that P_k defines a partial isometry, by imposing that the left TT cores are left-orthogonal while the right TT cores are right-orthogonal.

Lemma 2.2.3. *Let $(A_j)_{j \in [\![d]\!]}$ be a TT representation of some tensor $\boldsymbol{x} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$. For $k \in [\![d]\!]$, if $(A_1, \ldots, A_{k-1})$ is left-orthogonal and $(A_{k+1}, \ldots, A_d)$ is right-orthogonal, then P_k is a partial isometry.*

Proof. For $V \in \mathbb{R}^{r_{k-1} \times n_k \times r_k}$, we have

$$\begin{aligned}
\|P_k V\|^2 &= \sum_{i_1=1}^{n_1} \cdots \sum_{i_d=1}^{n_d} \operatorname{Tr}\big(X_d[i_d]^\mathsf{T} \cdots X_{k+1}[i_{k+1}]^\mathsf{T} V[i_k]^\mathsf{T} X_{k-1}[i_{k-1}]^\mathsf{T} \cdots X_1[i_1]^\mathsf{T} \\
&\qquad\qquad X_1[i_1] \cdots X_{k-1}[i_{k-1}] V[i_k] X_{k+1}[i_{k+1}] \cdots X_d[i_d]\big) \\
&= \sum_{i_1=1}^{n_1} \cdots \sum_{i_d=1}^{n_d} \operatorname{Tr}\big(V[i_k]^\mathsf{T} X_{k-1}[i_{k-1}]^\mathsf{T} \cdots X_1[i_1]^\mathsf{T} X_1[i_1] \cdots X_{k-1}[i_{k-1}] V[i_k] \\
&\qquad\qquad X_{k+1}[i_{k+1}] \cdots X_d[i_d] X_d[i_d]^\mathsf{T} \cdots X_{k+1}[i_{k+1}]^\mathsf{T}\big) \\
&= \sum_{i_k=1}^{n_k} \operatorname{Tr}\big(V[i_k]^\mathsf{T} V[i_k]\big) = \|V\|^2,
\end{aligned}$$

where we have used the cyclicity of the trace and the orthogonality of the TT cores. Thus P_k is indeed a partial isometry. □

The final algorithm is described in Algorithm 2.1, where at each step of the algorithm, we perform a linear solve for a reduced matrix $P_k^\mathsf{T} \boldsymbol{\mathcal{H}} P_k$ and a root shifting of the orthogonality center of the TT.

The optimisation steps (2.2.7) and (2.2.8) are called *microsteps*. An iteration over the loop s is called a sweep. Notice that at each microstep (2.2.7) or (2.2.8) the left TT cores are left-orthogonal and the right-TT cores are right-orthogonal, thanks to the root shifting step in the ALS algorithm.

2.2.2 Implementation details

In this part, we give some details about the implementation of the DMRG algorithm described in Algorithm 2.1, as well as the total computational cost of a sweep. Each microstep corresponds to solving a linear system of size $\mathcal{O}(nr^2)$ (where $n = \max n_k$ and $r = \max r_k$), hence at first glance, the storage cost would scale as $\mathcal{O}(n^2 r^4)$ and the computational cost of solving each linear system would scale as $\mathcal{O}(n^3 r^6)$ with a direct solver and $\mathcal{O}(n^2 r^4)$ for an iterative solver. Using the structure of the matrix $P_k^\mathsf{T} \boldsymbol{\mathcal{H}} P_k$, better scalings can be achieved.

Algorithm 2.1 One-site DMRG with sweeps

Input: $(X_1^{(0)}, \dots, X_d^{(0)})$ in right-orthogonal TT representation
Output: $(X_1^{(s)}, \dots, X_d^{(s)}) \in \mathscr{M}_{\mathrm{TT}_{\leq \mathbf{r}}}$ approximation of the minimiser in $\mathscr{M}_{\mathrm{TT}_{\leq \mathbf{r}}}$ of J

function ONE-SITE-DMRG($(X_1^{(0)}, \dots, X_d^{(0)})$)
$s = 0$
while `not converged` **do**
for $k = 1, 2, \dots, d-1$ **do** ▷ Forward half-sweep

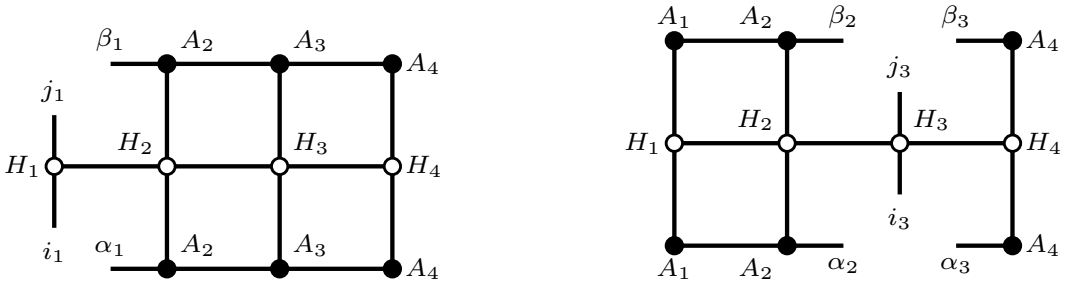
$$Y_k^{(s+\frac{1}{2})} = \underset{V_k \in \mathbb{R}^{r_{k-1} \times n_k \times r_k}}{\arg\min} j(X_1^{(s+\frac{1}{2})}, \dots, X_{k-1}^{(s+\frac{1}{2})}, V_k, X_{k+1}^{(s)}, \dots, X_d^{(s)}) \tag{2.2.7}$$

$Q, R = \mathtt{qr}\big(\big(Y_k^{(s+\frac{1}{2})}\big)_{\alpha_{k-1} i_k}^{\beta_k}\big)$ ▷ QR decomposition
$\big(X_k^{(s+\frac{1}{2})}[i_k]\big)_{\alpha_{k-1}}^{\alpha_k} = Q_{\alpha_{k-1} i_k}^{\alpha_k}$ ▷ Keep Q
$\big(X_{k+1}^{(s)}[i_{k+1}]\big)_{\alpha_k}^{\alpha_{k+1}} \leftarrow \big(R X_{k+1}^{(s)}[i_{k+1}]\big)_{\alpha_k}^{\alpha_{k+1}}$. ▷ Shift R to the right
end for
for $k = d, d-1, \dots, 2$ **do** ▷ Backward half-sweep

$$Y_k^{(s+1)} = \underset{V_k \in \mathbb{R}^{r_{k-1} \times n_k \times r_k}}{\arg\min} j(X_1^{(s+\frac{1}{2})}, \dots, X_{k-1}^{(s+\frac{1}{2})}, V_k, X_{k+1}^{(s+1)}, \dots, X_d^{(s+1)}) \tag{2.2.8}$$

$L, Q = \mathtt{lq}\Big(\big(Y_k^{(s+1)}\big)_{\alpha_{k-1}}^{\beta_k i_k}\Big)$ ▷ LQ decomposition
$\big(X_k^{(s+1)}[i_k]\big)_{\alpha_{k-1}}^{\alpha_k} = \big(Q\big)_{\alpha_{k-1}}^{\alpha_k i_k}$ ▷ Keep Q
$\big(X_{k-1}^{(s+\frac{1}{2})}[i_{k-1}]\big)_{\alpha_{k-2}}^{\alpha_{k-1}} \leftarrow \big(X_{k-1}^{(s+\frac{1}{2})}[i_{k-1}] L\big)_{\alpha_{k-2}}^{\alpha_{k-1}}$ ▷ Shift L to the left
end for
$s = s + 1$
end while
return $(X_1^{(s)}, \dots, X_d^{(s)})$
end function

The matrix $P_k^\mathsf{T}\boldsymbol{\mathcal{H}}P_k$ A critical step in DMRG is to efficiently implement the effective matrix $P_k^\mathsf{T}\boldsymbol{\mathcal{H}}P_k$ (see Figure 2.6).



(a) Effective matrix $(P_1^\mathsf{T}\boldsymbol{\mathcal{H}}P_1)^{\beta_1 j_1}_{\alpha_1 i_1} \in \mathbb{R}^{r_1 n_1 \times r_1 n_1}$

(b) Effective matrix $(P_3^\mathsf{T}\boldsymbol{\mathcal{H}}P_3)^{\beta_2 j_3 \beta_3}_{\alpha_2 i_2 \alpha_3} \in \mathbb{R}^{r_2 n_3 r_3 \times r_2 n_3 r_3}$

Figure 2.6: Examples of $P_k^\mathsf{T}\boldsymbol{\mathcal{H}}P_k$

As the TT ranks can be large (of the order of $10^3 - 10^4$), it is inefficient and useless to build the effective matrix $P_k^\mathsf{T}\boldsymbol{\mathcal{H}}P_k$. Instead, what is needed is the matrix-vector product $P_k^\mathsf{T}\boldsymbol{\mathcal{H}}P_k X_k$ where $X_k \in \mathbb{R}^{r_{k-1} n_k r_k}$. For this, a splitting of the effective Hamiltonian is used and it is written

$$\left(P_k^\mathsf{T}\boldsymbol{\mathcal{H}}P_k\right)^{\beta_{k-1} j_k \beta_k}_{\alpha_{k-1} i_k \alpha_k} = \sum_{\nu_k=1}^{R_k} \left(\boldsymbol{\mathcal{L}_k}\right)^{\beta_{k-1} j_k \nu_k}_{\alpha_{k-1} i_k} \left(\boldsymbol{\mathcal{R}_k}\right)^{\beta_k}_{\alpha_k \nu_k}. \tag{2.2.9}$$

This splitting is illustrated in Figure 2.7.

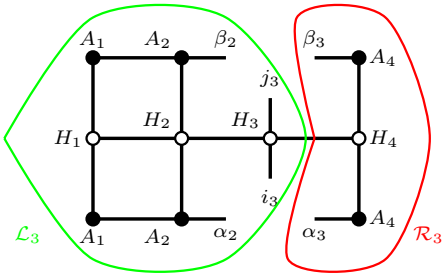


Figure 2.7: Splitting of the effective Hamiltonian

For iterative solvers, it is more relevant to focus on the computation of the matrix-vector multiplication. It goes as follows (see also Figure 2.8)

$$\left(P_k^\mathsf{T}\boldsymbol{\mathcal{H}}P_k\right)^{\beta_{k-1} j_k \beta_k}_{\alpha_{k-1} i_k \alpha_k} \left(X_k\right)_{\beta_{k-1} j_k \beta_k} = \left(\left(\boldsymbol{\mathcal{L}_k}\right)^{\beta_{k-1} j_k \nu_k}_{\alpha_{k-1} i_k} \left(X_k\right)_{\beta_{k-1} j_k \beta_k}\right) \left(\boldsymbol{\mathcal{R}_k}\right)^{\beta_k}_{\alpha_k \nu_k}, \tag{2.2.10}$$

i.e.

(i). first, we compute for $i_k \in [\![n_k]\!]$, $\nu_k \in [\![R_k]\!]$, $\alpha_{k-1} \in [\![r_{k-1}]\!]$, $\beta_k \in [\![r_k]\!]$ the sum

$$\sum_{\beta_{k-1}=1}^{r_{k-1}} \sum_{j_k=1}^{n_k} \left(\boldsymbol{\mathcal{L}_k}\right)_{\alpha_{k-1} i_k}^{\beta_{k-1} j_k \nu_k} \left(X_k\right)_{\beta_{k-1} j_k \beta_k}.$$

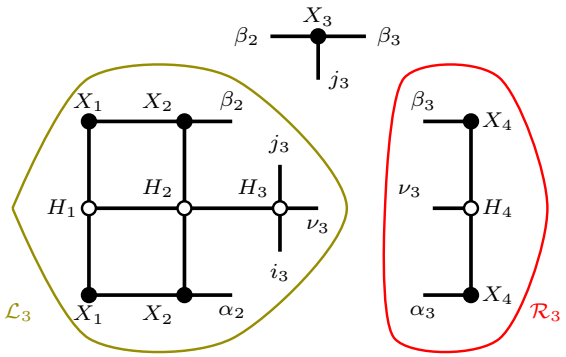
This scales as $\mathcal{O}(n^2 r^2 R)$.

(ii). in the second step, the previous tensor is contracted with $\boldsymbol{\mathcal{R}_k}$: for $\alpha_{k-1} \in [\![r_{k-1}]\!]$, $\alpha_k \in [\![r_k]\!]$, $i_k \in [\![n_k]\!]$, we sum

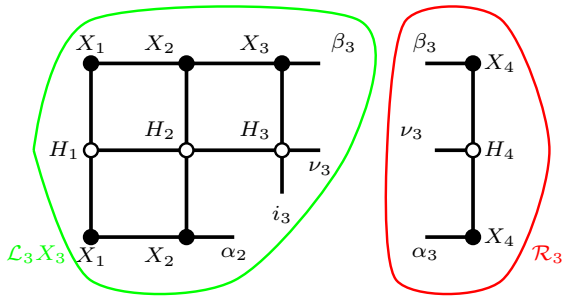
$$\sum_{\nu_k=1}^{R_k} \sum_{\beta_k=1}^{r_k} \left(\boldsymbol{\mathcal{L}_k} X_k\right)_{\alpha_{k-1} i_k \beta_k}^{\nu_k} \left(\boldsymbol{\mathcal{R}_k}\right)_{\alpha_k \nu_k}^{\beta_k}$$

This scales as $\mathcal{O}(n r^3 R)$.

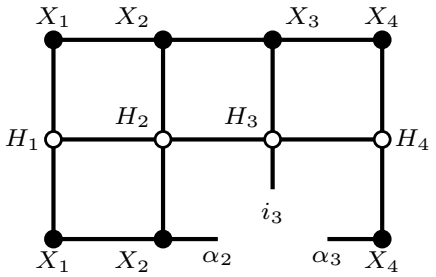
So overall the matrix-vector multiplication costs $\mathcal{O}(n^2 r^2 R + n r^3 R)$.



(a) Tensors $\boldsymbol{\mathcal{L}_3}$, X_3 and $\boldsymbol{\mathcal{R}_3}$

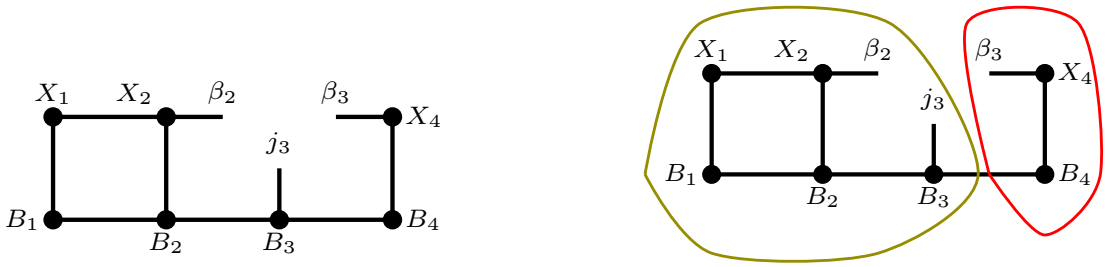


(b) First step in the matrix-vector product



(c) Result of the matrix-vector product

Figure 2.8: Matrix-vector product (2.2.10)



(a) $P_3^\mathsf{T}\boldsymbol{b}$ (b) Possible splitting of $P_3^\mathsf{T}\boldsymbol{b}$

Figure 2.9: Graphical representation of $P_3^\mathsf{T}\boldsymbol{b}$

The RHS $P_k^\mathsf{T}\boldsymbol{b}$ The assembly of the RHS is simpler than of the effective Hamiltonian. Similarly, it is possible to precompute the left and the right parts of the RHS as depicted in Figure 2.9b.

Operator updates The final main contribution to the total DMRG cost is the update of the effective Hamiltonians from one microstep to the next one. We would like to compute $\boldsymbol{\mathcal{L}_{k+1}}, \boldsymbol{\mathcal{R}_{k+1}}$ from $\boldsymbol{\mathcal{L}_k}, \boldsymbol{\mathcal{R}_k}$. In the case of a forward half-sweep, let us focus on the computation of $\boldsymbol{\mathcal{L}_{k+1}}$ from $\boldsymbol{\mathcal{L}_k}$. This can be done in 3 steps:

(i). as in the matrix-vector product we first compute for $i_k \in [\![n_k]\!], \nu_k \in [\![R_k]\!]$, $\alpha_{k-1} \in [\![r_{k-1}]\!], \beta_k \in [\![r_k]\!]$ the sum

$$\sum_{\beta_{k-1}=1}^{r_{k-1}} \sum_{j_k=1}^{n_k} \left(\boldsymbol{\mathcal{L}_k}\right)_{\alpha_{k-1} i_k}^{\beta_{k-1} j_k \nu_k} \left(X_k\right)_{\beta_{k-1} j_k \beta_k}.$$

This scales as $\mathcal{O}(n^2 r^2 R)$.

(ii). we then contract the result of the operation above with X_k, so for each $\alpha_k \in [\![r_k]\!]$, $\nu_k \in [\![R_k]\!]$, we need to compute the following sum

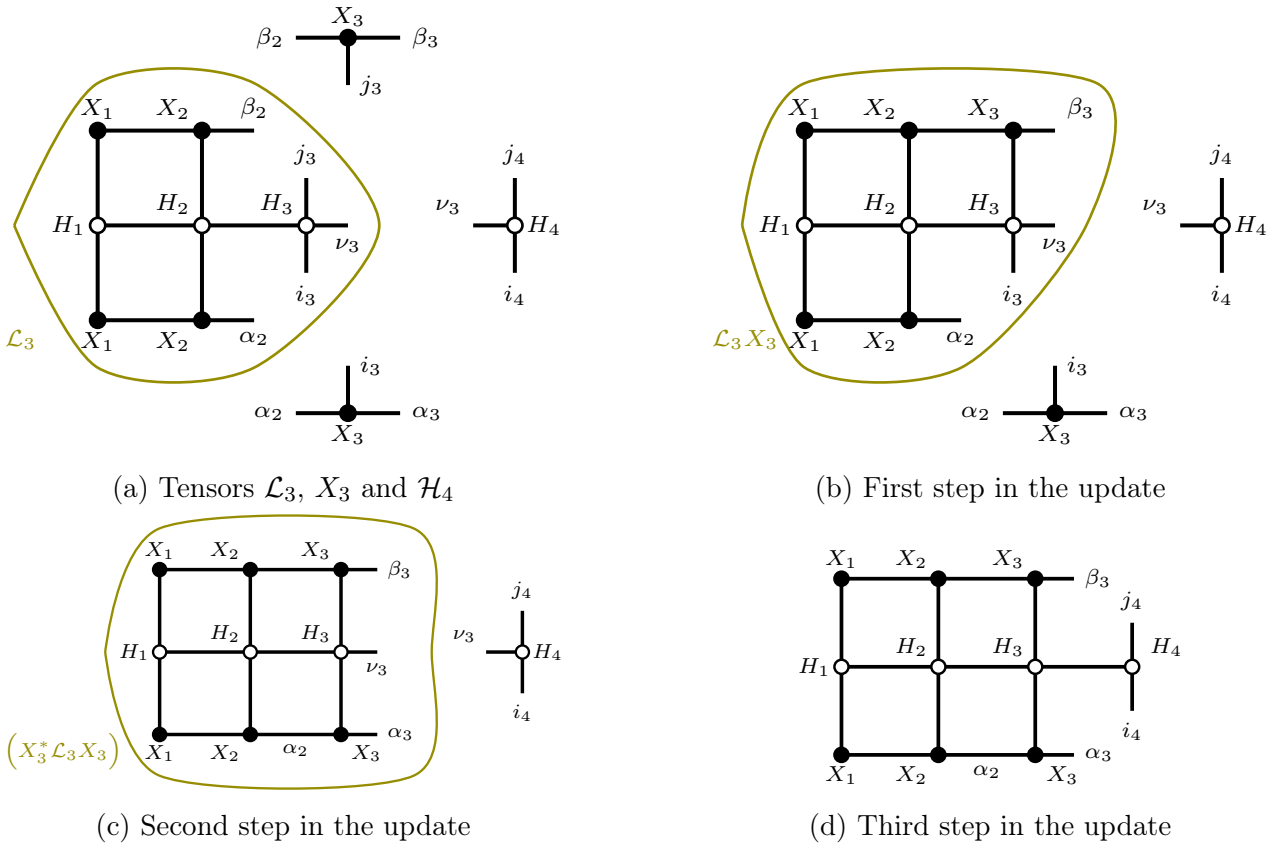
$$\sum_{\beta_{k-1}=1}^{r_{k-1}} \sum_{j_k=1}^{n_k} \left(\boldsymbol{\mathcal{L}_k} X_k\right)_{\alpha_{k-1} i_k \beta_k}^{\nu_k} \left(X_k\right)_{\alpha_{k-1} i_k \alpha_k}$$

This scales as $\mathcal{O}(n r^3 R)$.

(iii). finally, once the previous step is performed, one needs to contract with TTO core H_{k+1}, so for each $i_{k+1}, j_{k+1} \in [\![n_{k+1}]\!]$, $\nu_{k+1} \in [\![R_{k+1}]\!]$, $\alpha_k, \beta_k \in [\![r_k]\!]$, the following sum is computed

$$\sum_{\beta_{k-1}=1}^{r_{k-1}} \sum_{j_k=1}^{n_k} \left(X_k^\mathsf{T} \boldsymbol{\mathcal{L}_k} X_k\right)_{\alpha_k \beta_k}^{\nu_k} \left(H_{k+1}\right)_{\nu_k i_{k+1} j_{k+1} \nu_{k+1}}$$

This scales as $\mathcal{O}(n^2 r^2 R^2)$.



(a) Tensors $\mathcal{L}_3$, X_3 and $\mathcal{H}_4$

(b) First step in the update

(c) Second step in the update

(d) Third step in the update

Figure 2.10: Microstep operators updates

The cost of assembling $\boldsymbol{\mathcal{R}_k}$ from $\boldsymbol{\mathcal{R}_{k+1}}$ has the same scaling. The total cost of DMRG is summarised in the following Proposition.

Proposition 2.2.4 (Total cost of DMRG)**.** *The computational cost of DMRG scales as* $N_{\text{sweep}} d((n^2 r^2 R + n r^3 R) N_{\text{matvec}} + n^2 r^2 R^2)$*, where* N_{sweep} *is the number of total DMRG sweeps and* N_{matvec} *is the maximal number of matrix-vector products in all the microsteps.*

2.3 Convergence of DMRG

The global convergence of DMRG is a difficult problem, as the TT manifold is not a convex set. The convergence results on DMRG are local and assume that the Hessian of the functional j is of full-rank.

Assumption 2.3.1. *At the local minimiser* $\boldsymbol{x}_*$*, the Hessian* j'' *is of full rank*

$$\operatorname{rank} j''(\boldsymbol{x}_*) = \sum_{i=1}^{d} r_{i-1} n_i r_i - \sum_{i=1}^{d-1} r_i^2, \quad \textit{i.e. } \ker j''(\boldsymbol{x}_*) = T_{\boldsymbol{x}_*} \mathcal{M}_{\mathrm{TT}_{\leq r}}. \tag{2.3.1}$$

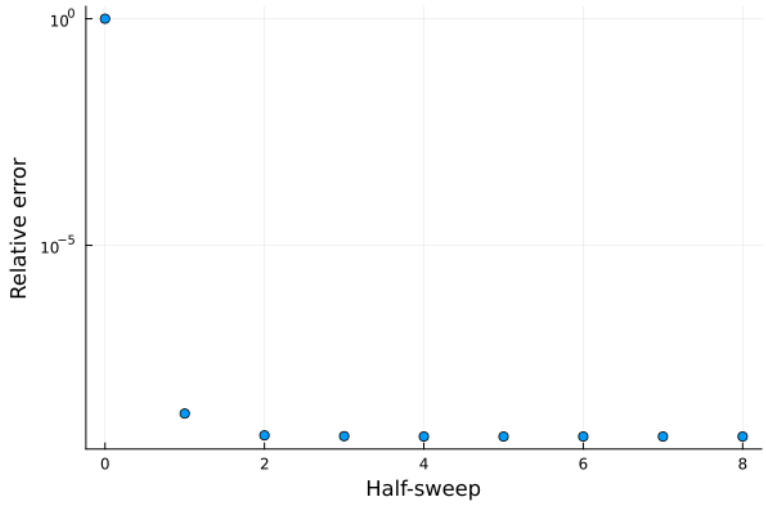


Figure 2.11: Convergence to the solution of $\boldsymbol{\mathcal{H}}\boldsymbol{x}_* = \boldsymbol{b}$ with $\boldsymbol{\mathcal{H}}$ the discrete Laplacian in $\mathbb{R}^{4^8\times 4^8}$, $\boldsymbol{b}$ a random tensor of TT rank 2. The reference solution has TT rank 10.

2.3.1 Local convergence of DMRG

Assumption 2.3.1 ensures that the Hessian is invertible at the solution to the DMRG equations.

Theorem 2.3.2 ([RU13, Theorem 2.7])**.** *Let $\boldsymbol{x}_*$ be a local minimiser of the problem (2.2.3). There exists a neighbourhood $\mathrm{W} \subset \mathscr{M}_{\mathrm{TT}_{\leq \mathbf{r}}}$ in $\mathscr{M}_{\mathrm{TT}_{\leq \mathbf{r}}}$ of $\boldsymbol{x}_*$ such that Algorithm 2.1 initiated with $\boldsymbol{x}^{(0)} \in \mathrm{W}$ converges to the minimiser $\boldsymbol{x}_*$.*

2.3.2 Half-sweep convergence

A more surprising result states that if the TT ranks in the DMRG algorithm are exactly the TT ranks of the sought solution, then DMRG returns the *exact* solution in a half-sweep (see Figure 2.11).

This result is shown in the case of $\boldsymbol{\mathcal{H}} = \mathrm{id}$ in [HRS12a].

Proposition 2.3.3 ([HRS12a, Lemma 4.2])**.** *Let $\boldsymbol{b} \in \mathbb{R}^{n_1\times\cdots\times n_d}$ with TT ranks $(r_0, \dots, r_d)$. Let $(B_1, \dots, B_d)$ be a left-orthogonal TT representation of $\boldsymbol{b}$. Let $(X_1, \dots, X_d)$ be a right-orthogonal TT with TT ranks $(r_0, \dots, r_d)$. Suppose that $(X_1, \dots, X_d)$ is such that for all $k \in [\![2; d]\!]$, the matrix $G_k \in \mathbb{R}^{r_{k-1}\times r_{k-1}}$ defined by*

$$\big(G_k\big)_{\beta_{k-1}\alpha_{k-1}} = \sum_{i_k,\dots,i_d} \sum_{\substack{\alpha_k\dots\alpha_{d-1}\\ \beta_k\dots\beta_{d-1}}} \big(X_k[i_k]\big)_{\alpha_{k-1}}^{\alpha_k} \cdots \big(X_d[i_d]\big)_{\alpha_{d-1}} \big(B_k[i_k]\big)_{\beta_{k-1}}^{\beta_k} \cdots \big(B_d[i_d]\big)_{\beta_{d-1}}.$$

is invertible. The DMRG algorithm applied with $H = \mathrm{id}$ converges in a half-sweep.

The condition on the initial guess is related to a nondeficiency of the initialisation of the DMRG algorithm.

Proof. We are going to prove by recurrence that there are $Q_k \in \mathbb{R}^{r_k \times r_k}$ for $k \in [\![d-1]\!]$ such that the solution of the DMRG microstep k can be written $X_k^{(\frac{1}{2})}[i_k] = Q_{k-1} B_k[i_k] Q_k^\mathsf{T}$.

Initialisation: since $(X_1, \dots, X_d)$ is right-orthogonal, we have that $P_1^\mathsf{T} P_1 = \mathrm{id}$. The solution to the first microstep is simply given by

$$Y_1[i_1]_{\alpha_1} = \sum_{\beta_1} B_1[i_1]_{\beta_1} (G_2)^{\beta_1}_{\alpha_1}.$$

Let Q_1^T, R_1 be the QR factorisation of G_2. Then

$$X_1^{(\frac{1}{2})}[i_1]_{\alpha_1} = \sum_{\beta_1} B_1[i_1]_{\beta_1} (Q_1)^{\alpha_1}_{\beta_1}.$$

Iteration: suppose that for all $j \in [\![k-1]\!]$, we have

$$X_j^{(\frac{1}{2})}[i_j]^{\alpha_{j-1}}_{\alpha_j} = \sum_{\beta_{j-1}, \beta_j} (Q_{j-1})^{\alpha_{j-1}}_{\beta_{j-1}} (B_j[i_j])^{\beta_{j-1}}_{\beta_j} (Q_j)^{\alpha_j}_{\beta_j}.$$

At microstep k, by left-orthogonality of $(X_j^{(\frac{1}{2})})_{1 \le j \le k-1}$ and right-orthogonality of $(X_j)_{k+1 \le j \le d}$, again the solution to the microstep k is given by

$$Y_k[i_k]^{\alpha_{k-1}}_{\alpha_k} = \sum_{\substack{\alpha_1 \dots \alpha_{k-1} \\ \beta_1 \dots \beta_k}} B_1[i_1]_{\beta_1} \cdots B_k[i_k]^{\beta_{k-1}}_{\beta_k} X_1^{(\frac{1}{2})}[i_1]_{\alpha_1} \cdots X_{k-1}^{(\frac{1}{2})}[i_{k-1}]^{\alpha_{k-2}}_{\alpha_{k-1}} (G_{k+1})^{\beta_k}_{\alpha_k}.$$

By the recurrence hypothesis and the orthogonality of the TT cores $(B_j)_{1 \le j \le k-1}$, the above expression simplifies to

$$Y_k[i_k]^{\alpha_{k-1}}_{\alpha_k} = \sum_{\beta_{k-1}, \beta_k} B_k[i_k]^{\beta_{k-1}}_{\beta_k} (Q_{k-1})^{\alpha_{k-1}}_{\beta_{k-1}} (G_{k+1})^{\beta_k}_{\alpha_k}.$$

Now let Q_k^T, R_k be the QR factorisation of G_{k+1}, then

$$X_k[i_k]^{\alpha_{k-1}}_{\alpha_k} = \sum_{\beta_{k-1}, \beta_k} (Q_{k-1})^{\alpha_{k-1}}_{\beta_{k-1}} B_k[i_k]^{\beta_{k-1}}_{\beta_k} (Q_k)^{\alpha_k}_{\beta_k},$$

which is exactly $X_k[i_k] = Q_{k-1} B_k[i_k] Q_k^\mathsf{T}$. This finishes the proof of the proposition. □

Remark 2.3.4. *A similar result holds for tensor rings, see [CLL20].*

2.4 Two-site DMRG: how to dynamically adapt the TT ranks

The main limitation of the one-site DMRG algorithm is the inability to dynamically adapt the TT ranks of the approximate solution during the course of the iterations. A small modification of the one-site DMRG makes it possible to have more flexibility in the TT ranks. The main idea is to solve the microstep in DMRG not only on one-site but on two neighbouring sites.

In that case, at each microstep k, the functional that is minimised is

$$j_2^{(k)} : \begin{cases} \mathbb{R}^{n_1 \times r_0 \times r_1} \times \cdots \times \mathbb{R}^{r_{k-1} \times n_k \times n_k \times r_{k+1}} \times \cdots \times \mathbb{R}^{n_d \times r_{d-1} \times r_d} \to \mathbb{R} \\ (X_1, \ldots, X_{k-1}, X, X_k, \ldots, X_d) \mapsto J \circ \widetilde{\mathrm{TT}}_k(X_1, \ldots, X_{k-1}, X, X_k, \ldots, X_d) \end{cases} \tag{2.4.1}$$

where

$$\widetilde{\mathrm{TT}}_k : \begin{cases} \mathbb{R}^{n_1 \times r_0 \times r_1} \times \cdots \times \mathbb{R}^{r_{k-1} \times n_k \times n_k \times r_{k+1}} \times \cdots \times \mathbb{R}^{n_d \times r_{d-1} \times r_d} \to \mathbb{R}^{n_1 \cdots n_d} \\ (X_1, \ldots, X_{k-1}, X, X_{k+1}, \ldots, X_d) \mapsto (X_1[i_1] \cdots X_{k-1}[i_{k-1}] X[i_k, i_{k+1}] X_{k+1}[i_{k+1}] \cdots X_d[i_d]). \end{cases}$$

The TT rank adaptivity comes in the transformation of the microstep solution back to a suitable TT form by a truncated SVD

$$(X^{\alpha_{k+1} i_{k+1}}_{\alpha_{k-1} i_k}) = U_\varepsilon S_\varepsilon V_\varepsilon^\mathsf{T} + \mathcal{O}(\varepsilon),$$

where $U_\varepsilon \in \mathbb{R}^{r_{k-1} n_k \times r}$, $S_\varepsilon \in \mathbb{R}^{r \times r}$ and $V_\varepsilon \in \mathbb{R}^{r_{k+1} n_{k+1} \times r}$ and r is chosen such that the truncated SVD has error ε. U_ε is (up to a reshape) the new TT core X_k and r is the corresponding TT rank. The full algorithm is given in Algorithm 2.2.

In practice, the truncation level ε is used to monitor the error in DMRG. It can also be used to extrapolate some quantities as the lowest eigenvalue as depicted in Figure 2.12 [WPAV14]. Theoretically, unlike the one-site algorithm, there is no convergence result on the two-site algorithm (except in the case where no truncation is made).

2.5 DMRG on eigenvalue problems

DMRG is primarily used to solve eigenvalue problems. In that case, the functional to minimise is $J(x) = \frac{\langle x, Hx \rangle}{\langle x, x \rangle}$. At each microstep, instead of solving a linear system, the following generalised eigenvalue problem has to be solved for the lowest eigenvalue

$$P_k^\mathsf{T} \boldsymbol{\mathcal{H}} P_k V = \lambda P_k^\mathsf{T} P_k V.$$

In that case, it is numerically beneficial to ensure the good orthogonality conditions for the approximate solution in the TT form, so that $P_k^\mathsf{T} P_k = \mathrm{id}$.

Apart from this change, the algorithms 2.1 and 2.2 can be modified in a straightforward way to solve eigenvalue problems instead.

For multiple lowest eigenvalues, there are two main options

Algorithm 2.2 Two-site DMRG with sweeps

Input: $(X_1^{(0)}, \dots, X_d^{(0)})$ in right-orthogonal TT representation with initial TT ranks $(r_0^{(0)}, \dots, r_d^{(0)})$, $\varepsilon_{\mathrm{TT}}$

Output: $(X_1^{(s)}, \dots, X_d^{(s)}) \in \mathscr{M}_{\mathrm{TT}_{\leq \mathbf{r}}}$ approximation of the minimiser of J

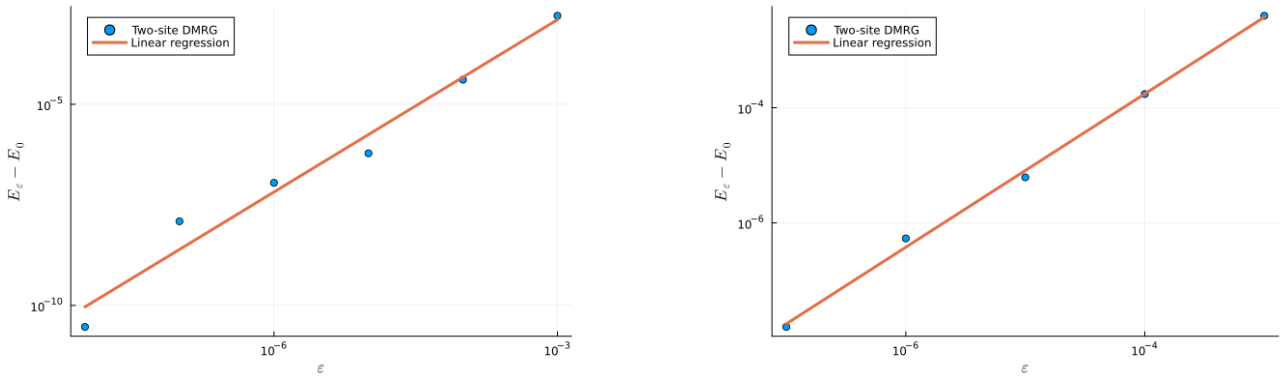
function TWO-SITE-DMRG($(X_1^{(0)}, \dots, X_d^{(0)}), \varepsilon_{\mathrm{TT}}$)
  $s = 0$
  while `not converged` **do**
    for $k = 1, 2, \dots, d-2$ **do** ▷ Forward half-sweep

$$Y_k^{(s+\frac{1}{2})} = \underset{V_k \in \mathbb{R}^{r_{k-1}^{(s+\frac{1}{2})} \times n_k \times n_k \times r_{k+1}^{(s)}}}{\arg\min} j_2^{(k)}(X_1^{(s+\frac{1}{2})}, \dots, X_{k-1}^{(s+\frac{1}{2})}, V_k, X_{k+2}^{(s)}, \dots, X_d^{(s)}) \tag{2.4.2}$$

      $U, S, V^{\mathsf{T}} = \mathtt{svd}_{\varepsilon_{\mathrm{TT}}}\big(\big(Y_k^{(s+\frac{1}{2})}\big)_{\alpha_{k-1} i_k}^{\beta_{k+1} i_{k+1}}\big)$ ▷ Truncated SVD of Y_k
      $r_k^{(s+\frac{1}{2})} =$ rank of the SVD truncation to level $\varepsilon_{\mathrm{TT}}$ ▷ Update TT rank
      $\big(X_k^{(s+\frac{1}{2})}[i_k]\big)_{\alpha_{k-1}}^{\alpha_k} = U_{\alpha_{k-1} i_k}^{\alpha_k}$ ▷ Update X_k
      $\big(X_{k+1}^{(s)}[i_{k+1}]\big)_{\alpha_k}^{\alpha_{k+1}} = \big(SV^{\mathsf{T}}\big)_{\alpha_k}^{\alpha_{k+1} i_{k+1}}$ ▷ Update X_{k+1}
    end for
    for $k = d-1, d-2, \dots, 2$ **do** ▷ Backward half-sweep

$$Y_k^{(s+1)} = \underset{V_k \in \mathbb{R}^{r_{k-2}^{(s+\frac{1}{2})} \times n_k \times n_k \times r_k^{(s+1)}}}{\arg\min} j_2^{(k)}(X_1^{(s+\frac{1}{2})}, \dots, X_{k-1}^{(s+\frac{1}{2})}, V_k, X_{k+2}^{(s+1)}, \dots, X_d^{(s+1)}) \tag{2.4.3}$$

      $U, S, V^{\mathsf{T}} = \mathtt{svd}_{\varepsilon_{\mathrm{TT}}}\big(\big(Y_k^{(s+\frac{1}{2})}\big)_{\alpha_{k-1} i_k}^{\beta_{k+1} i_{k+1}}\big)$ ▷ Truncated SVD of Y_k
      $r_k^{(s+1)} =$ rank of the SVD truncation to level $\varepsilon_{\mathrm{TT}}$ ▷ Update TT rank
      $\big(X_{k+1}^{(s+1)}[i_{k+1}]\big)_{\alpha_k}^{\alpha_{k+1}} = V_{\alpha_{k+1} i_{k+1}}^{\alpha_k}$ ▷ Update X_{k+1}
      $\big(X_k^{(s)}[i_k]\big)_{\alpha_{k-1}}^{\alpha_k} = \big(US\big)_{\alpha_{k-1} i_k}^{\alpha_k}$ ▷ Update X_k
    end for
    $s = s + 1$
  end while
  return $(X_1^{(s)}, \dots, X_d^{(s)})$
end function



(a) Hubbard model with 10 sites

(b) Hubbard model with 20 sites

Figure 2.12: Extrapolation of the ground-state energy E_ε for the Hubbard model where E_ε is computed with the two-site DMRG algorithm with truncation ε

(i). deflate the computed eigenvalues

(ii). use the following characterisation of the k smallest eigenvalues $(\lambda_1, \ldots, \lambda_k)$ of $\boldsymbol{\mathcal{H}}$

$$\sum_{i=1}^{k} \lambda_i = \min_{\boldsymbol{X} \in \mathbb{R}^{n_1 \cdots n_d \times k}} \frac{\mathrm{Tr}(\boldsymbol{X}^\mathsf{T} \boldsymbol{\mathcal{H}} \boldsymbol{X})}{\mathrm{Tr}(\boldsymbol{X}^\mathsf{T} \boldsymbol{X})}.$$

This approach is described in [DKOS14]. Essentially, the TT representing $\boldsymbol{X} \in \mathbb{R}^{n_1 \cdots n_d \times k}$ has an extra index accounting for the number of eigenvalues sought. At each microstep, this index is "moved" to the next microstep during the QR/SVD step.

Chapter 3

Low-rank representation of solutions to elliptic PDEs

In this chapter, we state results on the low-rank approximability for two types of problems

- source problems $\boldsymbol{\mathcal{H}u} = \boldsymbol{f}$;
- eigenvalue problems $\boldsymbol{\mathcal{H}u} = E\boldsymbol{u}$ for E the smallest eigenvalue of $\boldsymbol{\mathcal{H}}$,

where $\boldsymbol{\mathcal{H}}$ is a symmetric operator acting on the tensor space $\bigotimes_{j=1}^{d} \mathbb{R}^n$.

The main goal in this type of problems is to obtain an estimation of an approximate solution with TT ranks that do not depend exponentially with the dimension of the problem d, or on the quality of the approximation $\boldsymbol{u} - \boldsymbol{u}_{\text{approx}}$.

3.1 Source problems

For source problems, we will investigate the approximability by TT of the solution to the linear equation $\boldsymbol{\mathcal{H}u} = \boldsymbol{f}$ for operators of the form

$$\boldsymbol{\mathcal{H}} = \sum_{j=1}^{d} \boldsymbol{h}_j, \tag{3.1.1}$$

where $\boldsymbol{\mathcal{H}}$ is an operator acting on $\bigotimes_{j=1}^{d} \mathbb{R}^n$ and $\boldsymbol{h}_j$ is a one-body operator of the form $\mathrm{id}_{[\![j-1]\!]} \otimes h \otimes \mathrm{id}_{[\![j+1,d]\!]}$. Such operators $\boldsymbol{\mathcal{H}}$ will be referred to as *one-body operators* subsequently.

We are going to assume that h is a symmetric positive-definite matrix.

3.1.1 An approximation result by Chebyshev polynomials

With the assumption on h, the operator $\boldsymbol{\mathcal{H}}$ is symmetric positive-definite. Moreover, we know the lowest and the highest eigenvalues of $\boldsymbol{\mathcal{H}}$ from those of h. Let $\lambda_{\min}$ and $\lambda_{\max}$ be respectively

the lowest and largest eigenvalue of h. Then since $\boldsymbol{\mathcal{H}}$ is a one-body operator, it is diagonalisable in the tensor product of the eigenvectors of h. Thus we have that $d\lambda_{\min}$ is the lowest eigenvalue of $\boldsymbol{\mathcal{H}}$ and $d\lambda_{\max}$ its largest eigenvalue. This means that the condition number of $\boldsymbol{\mathcal{H}}$ is equal to $\frac{\lambda_{\max}}{\lambda_{\min}}$, *i.e.* the condition number of h. In particular, it is independent with respect to the dimension d. From this observation, we can deduce a bound on the TT rank of an approximation of the solution to the linear system $\boldsymbol{\mathcal{H}}\boldsymbol{u} = \boldsymbol{f}$.

Theorem 3.1.1 ([KU16])**.** *Let $\boldsymbol{\mathcal{H}}$ be a one-body operator,* i.e. *of the form*

$$\boldsymbol{\mathcal{H}} = \sum_{j=1}^{d} \boldsymbol{h}_j,$$

where $\boldsymbol{\mathcal{H}}$ is an operator acting on $\bigotimes_{j=1}^{d} \mathbb{R}^n$ and $\boldsymbol{h}_j$ is a one-body operator of the form $\mathrm{id}_{1:j-1} \otimes h \otimes \mathrm{id}_{j+1:d}$. Suppose that h is a symmetric positive-definite matrix. Let κ be the condition number of h. Let $\|\cdot\|_{\boldsymbol{\mathcal{H}}}$ be the norm on $\bigotimes_{j=1}^{d} \mathbb{R}^n$ be defined by

$$\forall x \in \bigotimes_{j=1}^{d} \mathbb{R}^n, \|x\|_{\boldsymbol{\mathcal{H}}}^2 = \frac{1}{d^2}\langle x, \boldsymbol{\mathcal{H}}x\rangle.$$

Let $f \in \bigotimes_{j=1}^{d} \mathbb{R}^n$ such that $\|f\| = 1$ and let $(f_I) \in \mathbb{R}^{d^n}$ be the coefficients of f in the canonical basis. Suppose that (f_I) has a TT representation with TT ranks bounded by r_f.

Then there exists a constant $C > 0$ independent of d for all $0 < \varepsilon < 2\|\boldsymbol{u}\|_{\boldsymbol{\mathcal{H}}}$, there is $\boldsymbol{u}_\varepsilon \in \bigotimes_{j=1}^{d} \mathbb{R}^n$ such that $\|\boldsymbol{u} - \boldsymbol{u}_\varepsilon\|_{\boldsymbol{\mathcal{H}}} \leq \varepsilon$ where $\boldsymbol{u}_\varepsilon$ has TT ranks bounded by

$$\frac{1}{2}\Big(\frac{C}{\sqrt{d}\,\varepsilon}\Big)^{1/\log_2(\frac{\sqrt{\kappa}+1}{\sqrt{\kappa}-1})} r_f$$

in the canonical basis of $\bigotimes_{j=1}^{d} \mathbb{R}^n$.

Proof. The proof relies on classical estimates for the solution of the linear system $\boldsymbol{\mathcal{H}}\boldsymbol{u} = \boldsymbol{f}$ where $\boldsymbol{\mathcal{H}}$ is symmetric positive-definite with Krylov methods.

In particular, we have a bound of the form

$$\|\boldsymbol{u} - \boldsymbol{u}^{(q)}\|_{\boldsymbol{\mathcal{H}}} \leq 2\Big(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\Big)^q \|\boldsymbol{u} - \boldsymbol{u}^{(0)}\|_{\boldsymbol{\mathcal{H}}},$$

where $\boldsymbol{u}^{(q)} = P_q(\boldsymbol{\mathcal{H}})(\boldsymbol{f} - \boldsymbol{\mathcal{H}}\boldsymbol{u}^{(0)})$ for some polynomial of degree q and κ is the condition number of $\boldsymbol{\mathcal{H}}$.

Selecting $\boldsymbol{u}^{(0)} = 0$, we have that the TT rank of such a $\boldsymbol{u}^{(q)}$ is bounded by $2^{q-1}r_f$ as $\boldsymbol{\mathcal{H}}$ has a TTO representation of rank 2. Hence to have $\|\boldsymbol{u} - \boldsymbol{u}^{(q)}\|_{\boldsymbol{\mathcal{H}}} \leq \varepsilon$, one needs

$$q \geq -\frac{\log_2\left(\frac{\varepsilon}{2\|\boldsymbol{u}\|_{\boldsymbol{\mathcal{H}}}}\right)}{\log_2\left(\frac{\sqrt{\kappa}+1}{\sqrt{\kappa}-1}\right)}.$$

Thus the TT rank of an approximation $\boldsymbol{u}_\varepsilon$ such that $\|\boldsymbol{u} - \boldsymbol{u}_\varepsilon\|_{\boldsymbol{\mathcal{H}}} \leq \varepsilon$ is bounded by $\frac{1}{2}\left(\frac{2\|\boldsymbol{u}\|_{\boldsymbol{\mathcal{H}}}}{\varepsilon}\right)^{1/\log_2(\frac{\sqrt{\kappa}+1}{\sqrt{\kappa}-1})} r_f$.

To finish the proof, we simply notice that

$$\|\boldsymbol{u}\|_{\boldsymbol{\mathcal{H}}}^2 = \langle \boldsymbol{u}, \boldsymbol{\mathcal{H}}\boldsymbol{u}\rangle = \langle \boldsymbol{u}, \boldsymbol{f}\rangle \leq \|\boldsymbol{u}\|\|\boldsymbol{f}\| \lesssim \frac{1}{\sqrt{d}}\|\boldsymbol{u}\|_{\boldsymbol{\mathcal{H}}}\|\boldsymbol{f}\|,$$

thus $\|\boldsymbol{u}\|_{\boldsymbol{\mathcal{H}}} \lesssim \frac{1}{\sqrt{d}}$.

This finishes the proof of this theorem. □

The bound on the ranks still depend on the local dimension n via the condition number of the matrix h, which for PDE discretisations grows with n. The next subsection deals with this issue.

3.1.2 An approximation result independent of the local dimension n

It is possible to derive a bound on the TT ranks that are independent of the local dimension n.

Theorem 3.1.2 ([DDGS16],[Bac23, Theorem 4.6]). *Let $\boldsymbol{\mathcal{H}}$ be a one-body operator,* i.e. *of the form*

$$\boldsymbol{\mathcal{H}} = \sum_{j=1}^{d} \boldsymbol{h}_j,$$

where $\boldsymbol{\mathcal{H}}$ is an operator acting on $\bigotimes_{j=1}^d \mathbb{R}^n$ and $\boldsymbol{h}_j$ is a one-body operator of the form $\mathrm{id}_{[\![j-1]\!]} \otimes h \otimes \mathrm{id}_{[\![j+1,d]\!]}$. Suppose that h is a symmetric positive-definite matrix with eigenvalues bounded from below by $\lambda > 0$.

Let $\boldsymbol{f} \in \bigotimes_{j=1}^d \mathbb{R}^n$ and $(f_I) \in \mathbb{R}^{n^d}$ be the coefficients of $\boldsymbol{f}$ in the canonical basis. Suppose that (f_I) has a TT representation with TT ranks bounded by r_f. Let $\boldsymbol{u} \in \bigotimes_{j=1}^d \mathbb{R}^n$ be the solution to $\boldsymbol{\mathcal{H}}\boldsymbol{u} = \boldsymbol{f}$.

Then for all $\varepsilon > 0$, there is $\boldsymbol{u}_\varepsilon \in \bigotimes_{j=1}^d \mathbb{R}^n$ such that $\|\boldsymbol{u} - \boldsymbol{u}_\varepsilon\| \leq \varepsilon$ where $\boldsymbol{u}_\varepsilon$ has TT ranks bounded by $\frac{1}{\pi^2}\log\left(\frac{d\lambda\varepsilon\|f\|}{16}\right)^2 r_f$ in the canonical basis of $\bigotimes_{j=1}^d \mathbb{R}^n$.

Remark 3.1.3. *The d-dimensional discrete Laplacian is a one-body operator of the form (3.1.1), hence for low-rank RHS, the solution to the linear problem has a low-rank approximation in the TT format.*

The main idea of the proof is to use the spectral decomposition of $\boldsymbol{\mathcal{H}}$ and an approximation of $1/x$ for $x > 0$ as a sum of exponentials:

$$\frac{1}{x} \approx \sum_{k=1}^{K} \omega_k e^{-\alpha_k x}, \text{ for some } \omega_k \in \mathbb{R} \text{ and } \alpha_k > 0. \tag{3.1.2}$$

Such an approximation can be obtained by noticing that for $x > 0$, we have

$$\frac{1}{x} = \int_0^\infty e^{-xt}\,\mathrm{d}t,$$

and using a quadrature rule for the integral.

Let $(\lambda_i, \phi_i) \in \mathbb{R} \times \mathbb{R}^n$ be the eigenpairs of h, then the eigenvalues Λ_I and the corresponding eigenvectors $\boldsymbol{\Phi}_I$ of $\boldsymbol{\mathcal{H}}$ are given by

$$\Lambda_I = \sum_{k=1}^{d} \lambda_{i_k}, \quad \boldsymbol{\Phi}_I = \phi_{i_1} \otimes \cdots \otimes \phi_{i_d}.$$

Then the solution to the linear system $\boldsymbol{\mathcal{H}}\boldsymbol{u} = \boldsymbol{f}$ is given by

$$\boldsymbol{u} = \sum_I \frac{1}{\Lambda_I} \tilde{f}_I \boldsymbol{\Phi}_I.$$

Since $\frac{1}{\Lambda_I}$ is not separable, the TT rank of $\boldsymbol{u}$ may be large. However it can be approximated by

$$\boldsymbol{u} = \sum_I \frac{1}{\Lambda_I} \tilde{f}_I \boldsymbol{\Phi}_I \approx \sum_{k=1}^{K} \sum_I \omega_k e^{-\alpha_k \Lambda_I} \tilde{f}_I \boldsymbol{\Phi}_I.$$

Now since $\Lambda_I = \sum_{j=1}^d \lambda_{i_j}$, we have that $e^{-\alpha_k \Lambda_I} = \prod_{j=1}^d e^{-\alpha_k \lambda_{i_j}}$, which is now separable in each variable. Thus the TT rank of the approximation of $\boldsymbol{u}$ is simply bounded by Kr_f.

The factor K is related to the quality of the approximation of $1/x$ by a sum of the exponential (3.1.2). For this problem, we have the following bound.

Proposition 3.1.4 ([Hac19],[Bac23, Corollary 4.5]). *Let $a > 0$. Then for all $K \in \mathbb{N}$, there are $\omega_k, \alpha_k > 0$, $1 \le k \le K$ such that*

$$\sup_{t \in [a,\infty)} \left| \frac{1}{x} - \sum_{k=1}^{K} \omega_k e^{-\alpha_k t} \right| \le \frac{16}{a} e^{-\pi\sqrt{K}}. \tag{3.1.3}$$

We can now give the proof of Theorem 3.1.2.

Proof of Theorem 3.1.2. Let $\widetilde{\boldsymbol{u}}$ be defined as

$$\widetilde{\boldsymbol{u}} = \sum_{k=1}^{K} \omega_k e^{-\alpha_k \boldsymbol{\mathcal{H}}} \boldsymbol{f},$$

where $(\omega_k), (\alpha_k)$ are chosen such that $\sup_{t \in [L\lambda,\infty)} \left| \frac{1}{x} - \sum_{k=1}^K \omega_k e^{-\alpha_k t} \right| \le \varepsilon$ with λ the smallest eigenvalue of h. This means that $K \ge \frac{1}{\pi^2} \log\left(\frac{d\lambda\varepsilon\|f\|}{16}\right)^2$. Then we have

$$\|\boldsymbol{u} - \widetilde{\boldsymbol{u}}\| \le \sup_{t \in [d\lambda,\infty)} \left| \frac{1}{x} - \sum_{k=1}^{K} \omega_k e^{-\alpha_k t} \right| \|\boldsymbol{f}\|.$$

For $K \geq \frac{1}{\pi^2} \log\left(\frac{d\lambda\varepsilon\|\boldsymbol{f}\|}{16}\right)^2$, we thus have $\|\boldsymbol{u} - \widetilde{\boldsymbol{u}}\| \leq \varepsilon$.

It remains to show that $\widetilde{\boldsymbol{u}}$ has TT ranks at most $\frac{1}{\pi^2} \log\left(\frac{d\lambda\varepsilon\|\boldsymbol{f}\|}{16}\right)^2 r_f$ in the basis of the eigenfunctions $(\boldsymbol{\Phi}_I)$ of $\boldsymbol{\mathcal{H}}$. As $\boldsymbol{\mathcal{H}} = \sum_{j=1}^d \boldsymbol{h}_j$ where $\boldsymbol{h}_j$ commute two-by-two, then $e^{-\alpha_k \boldsymbol{\mathcal{H}}} = \bigotimes_{j=1}^d e^{-\alpha_k h}$. Hence the TTO representation of $\bigotimes_{j=1}^d e^{-\alpha_k h}$ is of rank 1. Thus $e^{-\alpha_k \boldsymbol{\mathcal{H}}} \boldsymbol{f}$ has the same TT rank as $\boldsymbol{f}$. This finishes the proof. □

Remark 3.1.5. *The bound on the TT rank of the approximate solution does not depend on the dimension of the local space $\mathbb{R}^n$. We have thus the same bound at the continuous level for the ambient space norm. For elliptic operators, these bounds would be L^2 to L^2 bounds, however it would be more natural to have H^{-1} to H^1 bounds. With a more careful analysis, it is possible to obtain H^{-1+s} to H^1 bounds, with $s \in (0,1)$ (see [DDGS16, Prop. 1] or [Bac23, Thm. 4.6]). There is no proof in the critical case $s = 0$ of a low-rank approximation.*

3.2 Eigenvalue problems

Eigenvalue problems have attracted more attention as DMRG and tensor trains in general have been applied in the context of quantum physics, where the properties of the system are derived from the eigenvector associated to the lowest eigenvalue of the many-body operator.

The first rigorous work on the approximability of eigenvectors by low-rank TT is due to Hastings [Has07]. Later, another strategy of proof has been proposed by Arad et al. [AKLV13].

We restrict ourselves to results for two-body Hamiltonians with nearest neighbour interactions of the form

$$\boldsymbol{\mathcal{H}}^{(d)} = \sum_{j=1}^{d-1} \boldsymbol{W}_j \tag{3.2.1}$$

where $\boldsymbol{\mathcal{H}}^{(d)}$ is an operator acting on $\bigotimes_{j=1}^d \mathbb{R}^n$ and $\boldsymbol{W}_j$ is a two-body operator of the form $\mathrm{id}_{[\![j-1]\!]} \otimes W \otimes \mathrm{id}_{[\![j+2,d]\!]}$.

The main assumption needed to prove that the ground-state can be approximated well by a low-rank TT is the following.

Assumption 3.2.1. *Let $\boldsymbol{\mathcal{H}}^{(d)}$ be defined by (3.2.1). We assume that $\boldsymbol{\mathcal{H}}^{(d)}$ has a unique nondegenerate ground-state $\boldsymbol{\Psi}_0^{(d)}$ and that $\boldsymbol{\mathcal{H}}^{(d)}$ has a spectral gap γ independent of d,* i.e. *$E_1^{(d)} - E_0^{(d)} \geq \gamma$ for all d where $E_0^{(d)}$ and $E_1^{(d)}$ are the lowest and second lowest eigenvalue of $\boldsymbol{\mathcal{H}}^{(d)}$.*

The approximation result on the ground-state can be written as follows.

Theorem 3.2.2 ([Has07, AKLV13])**.** *Let $\boldsymbol{\mathcal{H}}^{(d)}$ be given by (3.2.1) satisfying Assumption 3.2.1. Then there is a function $r : (0,\infty) \to \mathbb{N}$ such for any $d \in \mathbb{N}$ and $\varepsilon > 0$, there is a TT approximation $\mathrm{TT}_{r(\varepsilon)} \boldsymbol{\Psi}_0^{(d)}$ with TT rank $r(\varepsilon)$ of $\boldsymbol{\Psi}_0^{(d)}$ such that*

$$\|\mathrm{TT}_{r(\varepsilon)} \boldsymbol{\Psi}_0^{(d)} - \boldsymbol{\Psi}_0^{(d)}\| \leq \varepsilon.$$

Remark 3.2.3. *Such approximation results are called* area laws *in physics. These approximation results in the physics litterature are usually written in terms of the ground-state projector* $|\boldsymbol{\Psi}_0^{(d)}\rangle\langle\boldsymbol{\Psi}_0^{(d)}|$ *which is an operator acting on* $\bigotimes_{j=1}^{d}\mathbb{R}^n$*. Looking at the partial trace of the ground-state projector on a block of neighbouring sites, it is possible to show that the approximation of the partial trace of the ground-state projector does not depend on the size of the block, but only on the "area" of the interaction, which in the case of the Hamiltonians considered here, is a constant. For interactions in higher dimension,* e.g. *on a 2D, 3D lattice, it is a folklore result that these types of result hold also for ground-state of nearest neighbour interactions Hamiltonians.*

3.2.1 Hastings area law

The full proof is given in Section 3.3 for the interested reader. We here give the essential ideas of the proof. First, we write an approximation of the projector onto the ground-state, using the energy gap assumption

$$|\boldsymbol{\Psi}_0^{(d)}\rangle\langle\boldsymbol{\Psi}_0^{(d)}| \approx \frac{1}{\sqrt{2\pi q}}\int_{\mathbb{R}} e^{\mathrm{i}(\boldsymbol{\mathcal{H}}^{(d)}-E_0)t}e^{-\frac{t^2}{2q}}\,\mathrm{d}t, \tag{3.2.2}$$

with q sufficiently large.

The Hamiltonian $\boldsymbol{\mathcal{H}}^{(d)}$ is a sum of operators that are "almost" commuting, as only neighbouring operators do not commute. Hence if $\boldsymbol{\mathcal{H}}_A = \sum_{j\in A}\boldsymbol{W}_j$, $\boldsymbol{\mathcal{H}}_{A^c} = \boldsymbol{\mathcal{H}} - \boldsymbol{\mathcal{H}}_A$ although we are not allowed to write $e^{i\boldsymbol{\mathcal{H}}^{(d)}t} = e^{i\boldsymbol{\mathcal{H}}_A t}e^{i\boldsymbol{\mathcal{H}}_{A^c}t}$, we can quantify the difference in a rigorous way. The trick is to write

$$e^{\mathrm{i}\boldsymbol{\mathcal{H}}^{(d)}t} = e^{\mathrm{i}\boldsymbol{\mathcal{H}}_{L+R}t+\mathrm{i}\boldsymbol{\mathcal{H}}_M t}e^{-\mathrm{i}\boldsymbol{\mathcal{H}}_{L+R}t}e^{\mathrm{i}\boldsymbol{\mathcal{H}}_{L+R}t},$$

with $\boldsymbol{\mathcal{H}}_M = \sum_{m-\ell\le j\le m+\ell}\boldsymbol{W}_j$, $\boldsymbol{\mathcal{H}}_{L+R} = \sum_{j<m-\ell;m+\ell<j}\boldsymbol{W}_j$ and realise that $e^{\mathrm{i}\boldsymbol{\mathcal{H}}_{L+R}t+\mathrm{i}\boldsymbol{\mathcal{H}}_M t}e^{-\mathrm{i}\boldsymbol{\mathcal{H}}_{L+R}t}$ is the solution to

$$\begin{cases}\mathrm{i}U'(t) = U(t)e^{\mathrm{i}\boldsymbol{\mathcal{H}}_{L+R}t}\boldsymbol{\mathcal{H}}_M e^{-\mathrm{i}\boldsymbol{\mathcal{H}}_{L+R}t}\\ U(0) = \mathrm{id}\,.\end{cases}$$

For small values of t by the Lieb-Robinson bound, proved for Hamiltonians with nearest neighbour interactions, $e^{\mathrm{i}\boldsymbol{\mathcal{H}}_{L+R}t}\boldsymbol{\mathcal{H}}_M e^{-\mathrm{i}\boldsymbol{\mathcal{H}}_{L+R}t}$ has support exponentially close to the support of $\boldsymbol{\mathcal{H}}_M$.

Denoting $\widetilde{U}_M(t) = e^{\mathrm{i}\boldsymbol{\mathcal{H}}_{L+R}t}\boldsymbol{\mathcal{H}}_M e^{-\mathrm{i}\boldsymbol{\mathcal{H}}_{L+R}t}$, we have then for small t

$$e^{\mathrm{i}\boldsymbol{\mathcal{H}}^{(d)}t} \approx \widetilde{U}_M(t)e^{\mathrm{i}\boldsymbol{\mathcal{H}}_{L+R}t},$$

with $\widetilde{U}_M(t)$ and $e^{\mathrm{i}\boldsymbol{\mathcal{H}}_{L+R}t}$ having exponentially small overlap.

3.2.2 AGSP

A later strategy to obtain these results have been through the *approximate ground-state projector* (AGSP) construction, first proposed in [AKLV13]. As opposed to the proof by Hastings,

where the central tool is the Lieb-Robinson bound, the AGSP is the result of an algorithm which terminates in finite time with polynomial complexity. This algorithm is called the *rigorous renormalisation group* (RRG) [RVM17]. It provides an alternative algorithm to DMRG for the computation of the ground-state energy. The scheme has been tested numerically in [RVM17, BMG+21], where RRG looked more stable than DMRG, but less efficient numerically. The other drawback of the RRG is that it is yet unclear how to adapt this algorithm to solve linear systems.

The idea of the proof uses a polynomial approximation of the ground-state projector. Indeed, because of the nearest neighbour interaction, the Hamiltonian $\boldsymbol{\mathcal{H}}^{(d)}$ has a TTO representation with ranks R independent of d. From algebraic properties of the TTO (see Chapter 2), the TTO representation of $P_n(\boldsymbol{\mathcal{H}})$ of degree n will have a TTO representation with TT ranks bounded by R^{n+1}.

Suppose that $\boldsymbol{\mathcal{H}}^{(d)}$ is of the form (3.2.1) such that it has a nondegenerate ground-state. The ground-state projector can be written

$$|\boldsymbol{\Psi}_0^{(d)}\rangle\langle\boldsymbol{\Psi}_0^{(d)}| \approx T_m(\boldsymbol{\mathcal{H}}),$$

where T_m is the rescaled Chebyshev polynomial of degree m such that $T_m(E_0) = 1$ and it is the solution to

$$\|T_m\|_\infty = \min_{P_m \in \mathbb{R}^m[X]} \max_{E_1 - E_0 \leq x \leq E_{\max} - E_0} |P_m(x)|.$$

The error on the approximation is bounded by

$$\| |\boldsymbol{\Psi}_0^{(d)}\rangle\langle\boldsymbol{\Psi}_0^{(d)}| - T_m(\boldsymbol{\mathcal{H}})\| \leq 2\Big(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\Big)^m,$$

where $\kappa = \frac{E_{\max}-E_0}{E_1-E_0}$. For this problem, typically $E_{\max} - E_0$ would scale as the number of tensorised spaces L but the gap would remain bounded. Hence to have $\| |\boldsymbol{\Psi}_0^{(d)}\rangle\langle\boldsymbol{\Psi}_0^{(d)}| - T_m(\boldsymbol{\mathcal{H}})\| \leq \varepsilon$, n would have to be of the order $\sqrt{d}\log(\varepsilon)$, thus the TTO rank of the approximate projector would be of the order $R^{\sqrt{d}}$, where R is the TTO rank of $\boldsymbol{\mathcal{H}}$.

This strategy does not beat the curse of dimension, because the norm of the operator scales as d. An additional ingredient is required to prove an area law like Theorem 3.2.2, which is a truncation of the high-frequency components of the Hamiltonian.

Let $\mathcal{J} \subset \{1, \dots, d\}$, $\boldsymbol{\mathcal{H}}_{\mathcal{J}} = \sum_{j\in\mathcal{J}} \boldsymbol{W}_j$ and $E_0^{\mathcal{J}}$ its ground-state eigenvalue. For $\tau > 0$, let $\Pi_{E_0^{\mathcal{J}}+\tau}$ be the spectral projector associated to the eigenvalues of $\boldsymbol{\mathcal{H}}_{\mathcal{J}}$ below $E_0^{\mathcal{J}} + \tau$ and $\Pi^{\perp}_{E_0^{\mathcal{J}}+\tau} = \mathrm{id} - \Pi_{E_0^{\mathcal{J}}+\tau}$. The truncated Hamiltonian on $\mathcal{J}$ is then defined by

$$\widetilde{\boldsymbol{\mathcal{H}}}_{\mathcal{J}} = \boldsymbol{\mathcal{H}}_{\mathcal{J}}\Pi_{E_0^{\mathcal{J}}+\tau} + (\tau + E_0^{\mathcal{J}})\Pi^{\perp}_{E_0^{\mathcal{J}}+\tau}. \tag{3.2.3}$$

By definition, $\|\widetilde{\boldsymbol{\mathcal{H}}}_{\mathcal{J}} - E_0^{\mathcal{J}}\| \leq \tau$.

The core idea of the proof is to establish the following result on the overlap between the ground-state of the full Hamiltonian $\boldsymbol{\mathcal{H}}^{(d)}$ and the projector onto the high-frequency components of a part of $\boldsymbol{\mathcal{H}}^{(d)}$.

Lemma 3.2.4 ([AKL16, Theorem 2.3]). *For $\mathcal{J} \subset \{1,\dots,d-1\}$, let $E_0^{\mathcal{J}}$ and $E_0^{(d)}$ be respectively the lowest eigenvalue of $\boldsymbol{\mathcal{H}}_{\mathcal{J}} = \sum_{j\in\mathcal{J}} \boldsymbol{W}_j$ and $\boldsymbol{\mathcal{H}}^{(d)}$. Let $E_0^{\mathcal{J}}$ be the lowest eigenvalue of $\boldsymbol{\mathcal{H}}_{\mathcal{J}}$. Let $\Pi_{[E_0^{\mathcal{J}}+E, E_0^{\mathcal{J}}+E']}$ be the spectral projector of $\boldsymbol{\mathcal{H}}_{\mathcal{J}}$ associated to the eigenvalues in $[E_0^{\mathcal{J}}+E, E_0^{\mathcal{J}}+E']$ $(E < E')$. Let $P_{[E_0^{(d)}, E_0^{(d)}+\varepsilon]}$ be the spectral projector of $\boldsymbol{\mathcal{H}}^{(d)}$ associated to the eigenvalues in $[E_0^{(d)}, E_0^{(d)}+\varepsilon]$. Then there are constants C and α independent of $E, E', \varepsilon, \mathcal{J}$ such that we have*

$$\|\Pi_{[E_0^{\mathcal{J}}+E, E_0^{\mathcal{J}}+E']} P_{[E_0^{(d)}, E_0^{(d)}+\varepsilon]}\| \leq C \exp\Big(-\alpha\big(E - \varepsilon + E_0^{\mathcal{J}} - E_0^{(d)}\big)\Big). \tag{3.2.4}$$

The proof of this lemma explicitly exploits the nearest neighbour interaction structure of the Hamiltonian $\boldsymbol{\mathcal{H}}^{(d)}$.

Sketch of the proof of Theorem 3.2.2 via AGSP

The proof of the area law requires a careful splitting of the Hamiltonian in two parts, such that the corresponding truncated Hamiltonian $\widetilde{\boldsymbol{\mathcal{H}}}_{\mathcal{J}}$ satisfies the following properties

(i). the ground-state of $\widetilde{\boldsymbol{\mathcal{H}}}_{\mathcal{J}}$ is exponentially close to $\boldsymbol{\Psi}_0^{(d)}$;

(ii). for a given cut k, the polynomial $T_m(\widetilde{\boldsymbol{\mathcal{H}}}_{\mathcal{J}})$ has a controlled TTO rank at the cut k.

We want to show the following result.

Proposition 3.2.5. *There is a constant $\alpha > 0$ such that for each $1 \leq k \leq d$ and all $\varepsilon > 0$, there is an approximation of the ground-state projector $|\boldsymbol{\Psi}_0^{(d)}\rangle\langle\boldsymbol{\Psi}_0^{(d)}|$ such that*

$$\||\boldsymbol{\Psi}_0^{(d)}\rangle\langle\boldsymbol{\Psi}_0^{(d)}| - \widetilde{P}_0\| \leq \varepsilon, \tag{3.2.5}$$

where $(\widetilde{P}_0)_{i_1\dots i_d}^{j_1\dots j_d} \in \mathbb{R}^{n^d\times n^d}$ such that its reshape $(\widetilde{P}_0)_{i_1 j_1,\dots,i_k j_k}^{i_{k+1} j_{k+1},\dots,i_d j_d} \in \mathbb{R}^{n^{2k}\times n^{2(d-k)}}$ has rank bounded by $CR^{\alpha(\log\varepsilon)^2}$ where R is the TTO rank of $\boldsymbol{\mathcal{H}}^{(d)}$ and C an irrelevant constant.

This means that the ground-state projector $|\boldsymbol{\Psi}_0^{(d)}\rangle\langle\boldsymbol{\Psi}_0^{(d)}|$ has a TTO approximation with error ε of TT rank $R^{\alpha(\log\varepsilon)^2}$. We then have the same bound on the TT approximation of the ground-state $\boldsymbol{\Psi}_0^{(d)}$.

Let $k \in [\![d-1]\!]$ and let $\widetilde{\boldsymbol{\mathcal{H}}}$ be the truncated Hamiltonian defined by

$$\widetilde{\boldsymbol{\mathcal{H}}} = \widetilde{\boldsymbol{\mathcal{H}}}_{\mathcal{J}} + \boldsymbol{\mathcal{H}}_{\mathcal{J}^c}, \tag{3.2.6}$$

where $\boldsymbol{\mathcal{H}}_{\mathcal{J}^c} = \sum_{k-\ell\leq j\leq k+\ell} \boldsymbol{W}_j$, $\boldsymbol{\mathcal{H}}_{\mathcal{J}} = \boldsymbol{\mathcal{H}} - \boldsymbol{\mathcal{H}}_{\mathcal{J}^c}$ and $\widetilde{\boldsymbol{\mathcal{H}}}_{\mathcal{J}} = \boldsymbol{\mathcal{H}}_{\mathcal{J}}\Pi_{E_0^{\mathcal{J}}+\tau} + (\tau + E_0^{\mathcal{J}})\Pi^{\perp}_{E_0^{\mathcal{J}}+\tau}$, with $\Pi_{E_0^{\mathcal{J}}+\tau}$ being the spectral projector of $\boldsymbol{\mathcal{H}}_{\mathcal{J}}$ with eigenvalues below $E_0^{\mathcal{J}} + \tau$. Let $\widetilde{\boldsymbol{\Psi}}_0$ be the ground-state of $\widetilde{\boldsymbol{\mathcal{H}}}$.

The proof has now two steps

(i). we show that $\||\boldsymbol{\Psi}_0^{(d)}\rangle\langle\boldsymbol{\Psi}_0^{(d)}| - |\widetilde{\boldsymbol{\Psi}}_0\rangle\langle\widetilde{\boldsymbol{\Psi}}_0|\| \leq C\exp(-\alpha(\tau - 2\ell))$

(ii). we prove that there is $\widetilde{P}_0$ such that $\||\widetilde{\boldsymbol{\Psi}}_0\rangle\langle\widetilde{\boldsymbol{\Psi}}_0| - \widetilde{P}_0\| \leq C\exp\Big(-\alpha\sqrt{\ell}\Big)$ for irrelevant constants α, C and where $\widetilde{P}_0$ has a reshape at the cut k with rank bounded by $R^{\ell+1}$.

Proof of step (i) The first step essentially follows from Lemma 3.2.4. Indeed we have

$$\|(\widetilde{\boldsymbol{\mathcal{H}}} - E_0)\boldsymbol{\Psi}_0^{(d)}\| = \|(\widetilde{\boldsymbol{\mathcal{H}}} - \boldsymbol{\mathcal{H}})\boldsymbol{\Psi}_0^{(d)}\| = \|(\boldsymbol{\mathcal{H}}_{\mathcal{J}} - \tau - E_0^{\mathcal{J}})\Pi_{E_0^{\mathcal{J}}+\tau}\boldsymbol{\Psi}_0^{(d)}\|.$$

Now we write

$$\begin{aligned}\|(\boldsymbol{\mathcal{H}}_{\mathcal{J}} - \tau - E_0^{\mathcal{J}})\Pi_{E_0^{\mathcal{J}}+\tau}\boldsymbol{\Psi}_0^{(d)}\| &\leq \sum_{k\geq 0}\|(\boldsymbol{\mathcal{H}}_{\mathcal{J}} - \tau - E_0^{\mathcal{J}})\Pi_{[\tau_{k+1},\tau_k]}\boldsymbol{\Psi}_0^{(d)}\| \\ &\leq C\exp\big(-\alpha(\tau - (E_0 - E_0^{\mathcal{J}}))\big)\sum_{k\geq 0}|\tau_k - \tau - E_0^{\mathcal{J}}|e^{-\alpha\tau_k},\end{aligned}$$

where we have used Lemma 3.2.4. Picking the right increasing sequence (τ_k), shows that

$$\|(\widetilde{\boldsymbol{\mathcal{H}}} - E_0)\boldsymbol{\Psi}_0^{(d)}\| \leq C\exp\big(-\alpha(\tau - (E_0 - E_0^{\mathcal{J}}))\big). \tag{3.2.7}$$

Using the positivity of the interactions $(\boldsymbol{W}_j)$, we have that $E_0 - E_0^{\mathcal{J}} \leq 2\|W\|\ell$. From usual estimates on approximate eigenpairs [Saa11, Theorem 3.9], we then have that

$$\||\boldsymbol{\Psi}_0^{(d)}\rangle\langle\boldsymbol{\Psi}_0^{(d)}| - |\widetilde{\boldsymbol{\Psi}}_0\rangle\langle\widetilde{\boldsymbol{\Psi}}_0|\| \leq \frac{\|(\widetilde{\boldsymbol{\mathcal{H}}} - E_0)\boldsymbol{\Psi}_0^{(d)}\|^2}{(\widetilde{E}_1 - E_0)^2} \leq C\exp(-\alpha(\tau - 2\ell)), \tag{3.2.8}$$

where $\widetilde{E}_1$ is the second lowest eigenvalue of $\widetilde{\boldsymbol{\mathcal{H}}}$ and where additionally one needs to prove that $\widetilde{E}_1 - E_0$ is bounded uniformly from below. This follows from Lemma 3.2.4 again and the spectral gap assumption 3.2.1. The proof is similar as to show that $\widetilde{E}_0 - E_0$ are close. This concludes the proof of the first step.

Proof of step (ii) Using the nearest neighbour nature of $\boldsymbol{W}_j$, we have that for $m < \ell$, $T_m(\widetilde{\boldsymbol{\mathcal{H}}})$ has a TTO rank bounded by $R^{\ell+1}$.

By definition of the truncated Hamiltonian $\widetilde{\boldsymbol{\mathcal{H}}}$, we have that $\|\widetilde{\boldsymbol{\mathcal{H}}} - E_0^{\mathcal{J}}\| \leq (2\ell\|W\| + \tau)$. By standard estimates of Chebyshev polynomials, we have that

$$\||\widetilde{\boldsymbol{\Psi}}_0\rangle\langle\widetilde{\boldsymbol{\Psi}}_0| - T_m(\widetilde{\boldsymbol{\mathcal{H}}})\| \leq 2\Big(\frac{\sqrt{\widetilde{\kappa}} - 1}{\sqrt{\widetilde{\kappa}} + 1}\Big)^m,$$

with $\widetilde{\kappa} = \frac{\widetilde{E}_{\max} - \widetilde{E}_0}{\widetilde{E}_1 - \widetilde{E}_0}$ where $\widetilde{E}_{\max}$ is the largest eigenvalue of $\widetilde{\boldsymbol{\mathcal{H}}}$ and $\widetilde{E}_0$, $\widetilde{E}_1$ the lowest and second lowest eigenvalue of $\widetilde{\boldsymbol{\mathcal{H}}}$.

From Eq. (3.2.7) and the gap assumption on the Hamiltonian $\boldsymbol{\mathcal{H}}$, we have that $\widetilde{\kappa} \leq C(\ell + \tau)$ for some constant C independent from $\widetilde{\boldsymbol{\mathcal{H}}}$. Hence we get

$$\||\widetilde{\boldsymbol{\Psi}}_0\rangle\langle\widetilde{\boldsymbol{\Psi}}_0| - T_m(\widetilde{\boldsymbol{\mathcal{H}}})\| \leq C\Big(1 - \frac{C}{\sqrt{\ell + \tau}}\Big)^m.$$

Choosing $\tau = \mathcal{O}(\ell)$ and noting that $(1 - \frac{a}{n})^n = \exp(-a) + o(1)$, we deduce that

$$\| |\widetilde{\mathbf{\Psi}}_0\rangle\langle\widetilde{\mathbf{\Psi}}_0| - T_{\ell-1}(\widetilde{\boldsymbol{\mathcal{H}}})\| \leq C \exp\Big(-C\sqrt{\ell}\Big). \tag{3.2.9}$$

Picking $\tau = 2\ell + \sqrt{\ell}$ and combining Eq. (3.2.8) and Eq. (3.2.9), we obtain

$$\| |\mathbf{\Psi}_0^{(d)}\rangle\langle\mathbf{\Psi}_0^{(d)}| - T_{\ell-1}(\widetilde{\boldsymbol{\mathcal{H}}})\| \leq C \exp\Big(-\alpha\sqrt{\ell}\Big), \tag{3.2.10}$$

where $T_{\ell-1}(\widetilde{\boldsymbol{\mathcal{H}}})$ has rank R^ℓ at cut k. This finishes the proof of Proposition 3.2.5.

3.3 Hastings area law

3.3.1 Hamiltonian with nearest neighbour interactions

The NNI Hamiltonian considered is of the form

$$\boldsymbol{\mathcal{H}}^{(d)} = \sum_{j=1}^{d-1} \boldsymbol{W}_j, \tag{3.3.1}$$

where $\boldsymbol{\mathcal{H}}^{(d)}$ is an operator acting on $\bigotimes_{j=1}^{d} \mathbb{RR}^n$ and $\boldsymbol{W}_j$ is a two-body operator of the form $\mathrm{id}_{[\![j-1]\!]} \otimes W \otimes \mathrm{id}_{[\![j+2,d]\!]}$.

Assumption 3.3.1. *We assume that for each d, the many-body Hamiltonian $\boldsymbol{\mathcal{H}}^{(d)}$ has a unique ground-state $\mathbf{\Psi}_0^{(d)}$ with eigenvalue 0 and a spectral gap $\gamma > 0$ independent of d.*

If the gap closes not too fast, it is possible to still get a polynomial bound on the TT approximation of the ground-state instead of an exponential one.

Remark 3.3.2. *Hastings' proof also holds if we relax the form of the two-body operators $\boldsymbol{W}_j$ to be such that $\mathrm{id}_{[\![j-1]\!]} \otimes W_j \otimes \mathrm{id}_{[\![j+2,d]\!]}$ with W_j acting on $\mathbb{R}^n \otimes \mathbb{R}^n$. In that case, if the operators $\boldsymbol{W}_j$ satisfy the following conditions*

- *the operators W_j are uniformly bounded, i.e. there is a constant C such that for all j, $\|W_j\| \leq C$;*
- *the commutators are uniformly bounded, i.e. there is a constant J such that for all j, $\|[W_j, W_{j+1}]\| \leq J$.*

The first assumption can actually be lifted and is taken for simplicity. As long as the commutators $[\widetilde{h}_j, \widetilde{h}_{j+1}]$ are uniformly bounded, the proof can be adapted to unbounded operators (see [Ali21]).

3.3.2 Lieb-Robinson bounds

An essential ingredient of the area law by Hastings is the repeated use of the Lieb-Robinson bound for NNI Hamiltonians. This bound describes how the correlation evolves for local operators.

Proposition 3.3.3 (Lieb-Robinson bound [NS06]). *Let $\boldsymbol{A} \in \mathscr{L}(\bigotimes_{i\in I} \mathbb{R}^n)$ and $\boldsymbol{B} \in \mathscr{L}(\bigotimes_{j\in J} \mathbb{R}^n)$ be two operators with $I \cap J = \varnothing$. Let $\boldsymbol{A}(t) = e^{\mathrm{i}\boldsymbol{\mathcal{H}}^{(d)}t}\boldsymbol{A} \otimes \mathrm{id}_{X^c}\, e^{-\mathrm{i}\boldsymbol{\mathcal{H}}^{(d)}t}$ with $\boldsymbol{\mathcal{H}}^{(d)}$ given by (3.3.1). Then there are constants $c, a, v > 0$ independent of $\boldsymbol{A}$, $\boldsymbol{B}$ or d such that*

$$\|[\boldsymbol{A}(t), \mathrm{id}_I \otimes \boldsymbol{B}]\| \leq c|I||J|\|\boldsymbol{A}\|\|\boldsymbol{B}\| \exp(-a(d(I,J) - v|t|)), \tag{3.3.2}$$

where $d(I,J) = \min_{i\in I, j\in J} |i-j|$.

The Lieb-Robinson bound is stated here in the special case of a one-dimensional NNI Hamiltonian but it holds for more general local interactions types [NS06]. In that case, the distance d is replaced by the natural distance of the interaction picture.

The Lieb-Robinson bound enables to state that the evolution of a local operator remains local by the next lemma.

Lemma 3.3.4. *Let $\boldsymbol{A} \in \mathscr{L}(\mathrm{X} \otimes \mathrm{Y})$. We assume that Y is finite-dimensional. Suppose there is $\varepsilon > 0$ such that for all $\boldsymbol{B} \in \mathscr{L}(\mathrm{Y})$, we have*

$$\|[\boldsymbol{A}, \mathrm{id}_{\mathrm{X}} \otimes \boldsymbol{B}]\| \leq \varepsilon \|\boldsymbol{B}\|. \tag{3.3.3}$$

Then there is an operator $\boldsymbol{A}_1 \in \mathscr{L}(\mathrm{X})$ such that

$$\|\boldsymbol{A} - \boldsymbol{A}_1 \otimes \mathrm{id}_{\mathrm{Y}}\| \leq \varepsilon. \tag{3.3.4}$$

Moreover, if $\boldsymbol{A}$ is self-adjoint, then $\boldsymbol{A}_1$ can also be chosen self-adjoint.

Proof of Lemma 3.3.4. The operator $\boldsymbol{A}_1$ is explicitely constructed: take $\boldsymbol{A}_1 = \frac{1}{\dim \mathrm{Y}} \mathrm{Tr}_{\mathrm{Y}} \boldsymbol{A} = \int_{\mathscr{U}(\mathrm{Y})} \mathrm{id}_{\mathrm{X}} \otimes U^* \boldsymbol{A}\, \mathrm{id} \otimes U \,\mathrm{d}U$ where $\mathrm{d}U$ is the uniform Haar measure on the unitary matrices of Y. Then we have

$$\|\boldsymbol{A} - \boldsymbol{A}_1 \otimes \mathrm{id}_{\mathrm{Y}}\| = \left\| \int_{\mathscr{U}(\mathrm{Y})} \mathrm{id}_{\mathrm{X}} \otimes U^* [\boldsymbol{A}, \mathrm{id} \otimes U] \,\mathrm{d}U \right\| \leq \varepsilon.$$

□

Corollary 3.3.5. *Let $\boldsymbol{A} \in \mathscr{L}(\bigotimes_{i\in I} \mathbb{R}^n)$, $\ell > 0$ and $\widetilde{I} = \{\tilde{i} \mid \exists i \in I, |i - \tilde{i}| \leq \ell\}$. Let $\boldsymbol{A}(t) = e^{\mathrm{i}\boldsymbol{\mathcal{H}}^{(d)}t}\boldsymbol{A} \otimes \mathrm{id}_{I^c}\, e^{-\mathrm{i}\boldsymbol{\mathcal{H}}^{(d)}t}$ with $\boldsymbol{\mathcal{H}}^{(d)}$ given by (3.3.1). Then for all $t \in \mathbb{R}$, there is an operator $\boldsymbol{A}_\ell(t) \in \mathscr{L}(\bigotimes_{i\in\widetilde{I}} \mathbb{R}^n)$ such that*

$$\|\boldsymbol{A}(t) - \boldsymbol{A}_\ell(t) \otimes \mathrm{id}_{\widetilde{I}^c}\| \leq d|I|\|\boldsymbol{A}\| \exp(-a(\ell - v|t|)). \tag{3.3.5}$$

If $\boldsymbol{A}$ is self-adjoint, then $\boldsymbol{A}_\ell(t)$ is self-adjoint for all t.

Proof. Combining Lemma 3.3.4 with the Lieb-Robinson bonud (3.3.2), we directly get the result. □

3.3.3 Main theorem and Hastings area law

The main result in Hastings seminal paper states that the ground-state projector can be exponentially well approximated using an almost tensor product of operators with an overlapping domain of size ℓ independent of the size of the system.

Theorem 3.3.6. *Let $\boldsymbol{\mathcal{H}}^{(d)}$ be the Hamiltonian defined in (3.3.1) satisfying the assumptions 3.3.1. For any $1 \leq j \leq d$ and any $\ell \geq 0$, there are operators $O_L \in \mathscr{L}(\mathcal{H}_{1:j})$, $O_M \in \mathscr{L}(\mathcal{H}_{j-\ell:j+\ell})$ and $O_R \in \mathscr{L}(\mathcal{H}_{j+1:d})$ with $\|O_M\|, \|O_L\|, \|O_R\| \leq 1$ and there is $\beta > 0$ independent of ℓ and d and $C > 0$ depending polynomially on d such that*

$$\left\|(\mathrm{id}_{1:j-\ell-1} \otimes O_M \otimes \mathrm{id}_{j+\ell+1:d})(O_L \otimes \mathrm{id}_{j+1:d})(\mathrm{id}_{1:j} \otimes O_R) - |\boldsymbol{\Psi}_0^{(d)}\rangle\langle\boldsymbol{\Psi}_0^{(d)}|\right\| \leq C \exp(-\beta\ell). \quad (3.3.6)$$

From eq. (3.3.6), the area law and the TT approximation of the ground-state follows.

Corollary 3.3.7. *Let $\boldsymbol{\Psi}_0^{(d)}$ be the ground-state wave function of $\boldsymbol{\mathcal{H}}^{(d)}$ given by (3.3.1). Then the following assertions are true:*

(i). there is a constant S independent of L such that $S_\alpha(|\boldsymbol{\Psi}_0^{(d)}\rangle\langle\boldsymbol{\Psi}_0^{(d)}|) \leq S$;

(ii). for any $\varepsilon > 0$, there is a TT approximation $\mathrm{TT}_r \boldsymbol{\Psi}_0^{(d)}$ with TT rank r independent of d of $\boldsymbol{\Psi}_0^{(d)}$ such that

$$\|\mathrm{TT}_r \boldsymbol{\Psi}_0^{(d)} - \boldsymbol{\Psi}_0^{(d)}\| \leq \varepsilon.$$

Remark 3.3.8. *It is possible to choose the operators O_L, O_M and O_R to be nonnegative. By construction, O_L and O_R are nonnegative and by a little trick, O_M can also be chosen nonnegative [Has07].*

Sketch of an almost-proof of Theorem 3.3.6 The proof of the theorem relies on the following approximation of the ground-state projection

$$\rho_q = \frac{1}{\sqrt{2\pi q}} \int_{\mathbb{R}} e^{\mathrm{i}\boldsymbol{\mathcal{H}}^{(d)} t} e^{-\frac{t^2}{2q}} \,\mathrm{d}t, \quad (3.3.7)$$

where $q > 0$ is fixed later on. Using the spectral gap assumption, we see that

$$\|\rho_q - |\boldsymbol{\Psi}_0^{(d)}\rangle\langle\boldsymbol{\Psi}_0^{(d)}|\| \leq e^{-\frac{1}{2}\gamma^2 q}, \quad (3.3.8)$$

where γ is the spectral gap.

Using the NNI structure of the Hamiltonian, we can write

$$H = H_{L+R} + H_M,$$

with $H_M = \sum_{k=j-\frac{\ell}{2}}^{j+\frac{\ell}{2}} h_k$ and $H_{L+R} = \sum_{k<j-\frac{\ell}{2}} h_k + \sum_{k>j+\frac{\ell}{2}} h_k$. The evolution $e^{\mathrm{i}\boldsymbol{\mathcal{H}}^{(d)}t}$ can be written

$$e^{\mathrm{i}\boldsymbol{\mathcal{H}}^{(d)}t} = e^{\mathrm{i}H_{L+R}t+\mathrm{i}H_M t}e^{-\mathrm{i}H_{L+R}t}e^{\mathrm{i}H_{L+R}t}.$$

The trick is to realise that $e^{\mathrm{i}H_{L+R}t+\mathrm{i}H_M t}e^{-\mathrm{i}H_{L+R}t}$ is the solution to

$$\begin{cases} \mathrm{i}U'(t) = U(t)e^{\mathrm{i}H_{L+R}t}H_M e^{-\mathrm{i}H_{L+R}t} \\ U(0) = \mathrm{id}\,. \end{cases}$$

Since $H_M = \mathrm{id}_{1:j-\frac{\ell}{2}} \otimes \tilde{H}_M \otimes \mathrm{id}_{j+\frac{\ell}{2}+1:d}$, using Corollary 3.3.5, then for all $t \in \mathbb{R}$, there is $H_M^{(\ell)}(t) \in \mathscr{L}(\mathcal{H}_{j-\ell:j+\ell})$ such that

$$\left\| e^{\mathrm{i}H_{L+R}t}H_M e^{-\mathrm{i}H_{L+R}t} - \mathrm{id}_{1:j-\ell-1} \otimes H_M^{(\ell)}(t) \otimes \mathrm{id}_{j+\ell+1:d} \right\| \leq 2d\ell\|H_M\| \exp\bigl(-a(\tfrac{\ell}{2} - v|t|)\bigr).$$

Thus the operator $e^{\mathrm{i}H_{L+R}t+\mathrm{i}H_M t}e^{-\mathrm{i}H_{L+R}t}$ can be approximated by

$$e^{\mathrm{i}H_{L+R}t+\mathrm{i}H_M t}e^{-\mathrm{i}H_{L+R}t} = \mathcal{T}\exp\Bigl(\int_0^t \mathrm{id}_{1:j-\ell-1} \otimes H_M^{(\ell)}(\tau) \otimes \mathrm{id}_{j+\ell+1:d}\,\mathrm{d}\tau\Bigr)^*,$$

where for an operator $A(t)$, $\mathcal{T}\exp\bigl(\int_0^t A(\tau)\,\mathrm{d}\tau\bigr)$ is the time-ordered exponential defined by [RS75, Chapter X.12]

$$\mathcal{T}\exp\Bigl(\int_0^t A(\tau)\,\mathrm{d}\tau\Bigr) = \lim_{N\to\infty} e^{A(t_N)\Delta t}e^{A(t_{N-1})\Delta t}\cdots e^{A(t_1)\Delta t}, \quad t_k = k\Delta t, \quad \Delta t = \frac{t}{N}.$$

Using a Duhamel formula, the approximation of the ground-state projector is

$$\begin{aligned} |\boldsymbol{\Psi}_0^{(d)}\rangle\langle\boldsymbol{\Psi}_0^{(d)}| &= \frac{1}{\sqrt{2\pi q}}\int_{\mathbb{R}} e^{\mathrm{i}\boldsymbol{\mathcal{H}}^{(d)}t}e^{-\frac{t^2}{2q}}\,\mathrm{d}t + \mathcal{O}(e^{-\frac{1}{2}\gamma^2 q}) \\ &= \frac{1}{\sqrt{2\pi q}}\int_{\mathbb{R}} \mathcal{T}\exp\Bigl(\int_0^t \mathrm{id}_{1:j-\ell-1} \otimes H_M^{(\ell)}(\tau) \otimes \mathrm{id}_{j+\ell+1:d}\,\mathrm{d}\tau\Bigr)^* e^{\mathrm{i}H_{L+R}t}e^{-\frac{t^2}{2q}}\,\mathrm{d}t \\ &\qquad + \mathcal{O}(e^{-\frac{1}{2}\gamma^2 q} + q^{3/2}e^{-a\ell}). \end{aligned}$$

We would be done if it were possible to write $e^{\mathrm{i}H_{L+R}t} \simeq O_L \otimes \mathrm{id}_{j+1:d}\,\mathrm{id}_{1:j} \otimes O_R$ for $O_L \in \mathscr{L}(\mathcal{H}_{1:j})$ and $O_R \in \mathscr{L}(\mathcal{H}_{j+1:d})$ that are independent of t. In order to do so, another transformation is applied to H_M and H_{L+R} to guarantee that such a step is justified.

Proof of Theorem 3.3.6

Lemma 3.3.9. *Let $q > 0$ and ρ_q be defined by*

$$\rho_q = \frac{1}{\sqrt{2\pi q}} \int_{\mathbb{R}} e^{\mathrm{i}\boldsymbol{\mathcal{H}}^{(d)} t} e^{-\frac{t^2}{2q}} \, \mathrm{d}t. \tag{3.3.9}$$

Then we have

$$\|\rho_q - |\boldsymbol{\Psi}_0^{(d)}\rangle\langle\boldsymbol{\Psi}_0^{(d)}|\| \leq e^{-\frac{1}{2}\gamma^2 q}, \tag{3.3.10}$$

where γ is the spectral gap.

Proof. This follows from the spectral gap assumption 3.3.1 and the fact that the Fourier transform of $t \mapsto \frac{1}{\sqrt{2\pi q}} e^{-\frac{t^2}{2q}}$ is $\omega \mapsto e^{-\frac{1}{2}\omega^2}$. □

Lemma 3.3.10. *For $1 \leq j \leq d$ and $\ell > 0$, let*

$$H_M = \sum_{k=j-\frac{\ell}{3}}^{j+\frac{\ell}{3}} h_k, \quad H_L = \sum_{k<j-\frac{\ell}{3}} h_k, \quad H_R \sum_{k>j+\frac{\ell}{3}} h_k.$$

For $q > 0$, let

$$H_M(q) = \frac{1}{\sqrt{2\pi q}} \int_{\mathbb{R}} e^{-\mathrm{i}\boldsymbol{\mathcal{H}}^{(d)} t} H_M e^{\mathrm{i}\boldsymbol{\mathcal{H}}^{(d)} t} e^{-\frac{t^2}{2q}} \, \mathrm{d}t - \langle \boldsymbol{\Psi}_0^{(d)}, H_M \boldsymbol{\Psi}_0^{(d)} \rangle \tag{3.3.11}$$

$$H_L(q) = \frac{1}{\sqrt{2\pi q}} \int_{\mathbb{R}} e^{-\mathrm{i}\boldsymbol{\mathcal{H}}^{(d)} t} H_L e^{\mathrm{i}\boldsymbol{\mathcal{H}}^{(d)} t} e^{-\frac{t^2}{2q}} \, \mathrm{d}t - \langle \boldsymbol{\Psi}_0^{(d)}, H_L \boldsymbol{\Psi}_0^{(d)} \rangle \tag{3.3.12}$$

$$H_R(q) = \frac{1}{\sqrt{2\pi q}} \int_{\mathbb{R}} e^{-\mathrm{i}\boldsymbol{\mathcal{H}}^{(d)} t} H_R e^{\mathrm{i}\boldsymbol{\mathcal{H}}^{(d)} t} e^{-\frac{t^2}{2q}} \, \mathrm{d}t - \langle \boldsymbol{\Psi}_0^{(d)}, H_R \boldsymbol{\Psi}_0^{(d)} \rangle. \tag{3.3.13}$$

Then for all $q > 0$, we have

$$H = H_L(q) + H_M(q) + H_R(q), \tag{3.3.14}$$

and

$$\|H_M(q)\boldsymbol{\Psi}_0^{(d)}\|, \|H_L(q)\boldsymbol{\Psi}_0^{(d)}\|, \|H_R(q)\boldsymbol{\Psi}_0^{(d)}\| \leq \gamma J e^{-\frac{1}{2}\gamma^2 q}. \tag{3.3.15}$$

Proof. Since $H = H_L + H_M + H_R$, eq. (3.3.14) is clear. For eq. (3.3.15), we have

$$\begin{aligned} H_M(q)\boldsymbol{\Psi}_0^{(d)} &= \frac{1}{\sqrt{2\pi q}} \int_{\mathbb{R}} e^{-\mathrm{i}\boldsymbol{\mathcal{H}}^{(d)} t} H_M e^{\mathrm{i}\boldsymbol{\mathcal{H}}^{(d)} t} \boldsymbol{\Psi}_0^{(d)} e^{-\frac{t^2}{2q}} \, \mathrm{d}t - \langle \boldsymbol{\Psi}_0^{(d)}, H_M \boldsymbol{\Psi}_0^{(d)} \rangle \boldsymbol{\Psi}_0^{(d)} \\ &= \frac{1}{\sqrt{2\pi q}} \int_{\mathbb{R}} e^{-\mathrm{i}\boldsymbol{\mathcal{H}}^{(d)} t} P_0^{\perp} H_M \boldsymbol{\Psi}_0^{(d)} e^{-\frac{t^2}{2q}} \, \mathrm{d}t, \end{aligned}$$

where $P_0^\perp = \mathrm{id} - |\mathbf{\Psi}_0^{(d)}\rangle\langle\mathbf{\Psi}_0^{(d)}|$. We have

$$\|P_0^\perp H_M \mathbf{\Psi}_0^{(d)}\| \leq \gamma \|H H_M \mathbf{\Psi}_0^{(d)}\| \leq \gamma \|[H, H_M]\mathbf{\Psi}_0^{(d)}\| \leq \gamma J.$$

Hence using again the spectral gap of $\boldsymbol{\mathcal{H}}^{(d)}$, we obtain

$$\|H_M(q)\mathbf{\Psi}_0^{(d)}\| \leq \gamma J e^{-\frac{1}{2}\gamma^2 q}. \tag{3.3.16}$$

The same proof applies to H_L and H_R. □

The operators $H_L(q)$, $H_M(q)$ and $H_R(q)$ do not have the same support as H_L, H_M and H_R. In fact, their support is now the full Hilbert space $\mathcal{H}_{1:d}$. However, this can be solved by truncating the operators using Corollary 3.3.5.

Lemma 3.3.11. *There are self-adjoint operators $\widetilde{H}_L(q)$, $\widetilde{H}_M(q)$ and $\widetilde{H}_R(q)$ with respective support in $\mathcal{H}_{1:j}$, $\mathcal{H}_{j-2\ell/3:j+2\ell/3}$ and $\mathcal{H}_{j+1:d}$ such that*

$$\begin{aligned}
\|H_M(q) - \widetilde{H}_M(q)\| &\lesssim \|h\|\ell^2 d e^{-a\ell/3} e^{qa^2v^2/2}, \\
\|H_L(q) - \widetilde{H}_L(q)\| &\lesssim \|h\|\ell^2 d e^{-a\ell/3} e^{qa^2v^2/2}, \\
\|H_R(q) - \widetilde{H}_R(q)\| &\lesssim \|h\|\ell^2 d e^{-a\ell/3} e^{qa^2v^2/2}.
\end{aligned}$$

Proof. We only give the proof for $\widetilde{H}_M(q)$ as it is identical for the other truncations. By Corollary 3.3.5, there is an operator $H_M^{(\ell)}(t)$ with support in $\mathcal{H}_{j-2\ell/3:j+2\ell/3}$ such that

$$\|e^{-\mathrm{i}\boldsymbol{\mathcal{H}}^{(d)}t} H_M e^{\mathrm{i}\boldsymbol{\mathcal{H}}^{(d)}t} - H_M^{(\ell)}(t)\| \leq \|h\|\ell^2 d \exp(-a(\ell/3 - v|t|)).$$

Using that for $p, q > 0$, $\int_0^\infty e^{pt} e^{-\frac{t^2}{2q}}\,\mathrm{d}t \lesssim q^{1/2} e^{p^2 q/2}$.We deduce that there is an operator $\widetilde{H}_M(q)$ such that

$$\|H_M(q) - \widetilde{H}_M(q)\| \lesssim \|h\|\ell^2 d e^{-a\ell/3} e^{qa^2v^2/2}.$$

□

Lemma 3.3.12. *Let $q > 0$ and $\widetilde{\rho}_q$ be given by*

$$\widetilde{\rho}_q = \frac{1}{\sqrt{2\pi q}} \int_{\mathbb{R}} e^{\mathrm{i}(\widetilde{H}_L(q) + \widetilde{H}_M(q) + \widetilde{H}_R(q))t} e^{-\frac{t^2}{2q}}\,\mathrm{d}t,$$

where $\widetilde{H}_L(q)$, $\widetilde{H}_M(q)$ and $\widetilde{H}_R(q)$ are defined in Lemma 3.3.11. Then we have

$$\left\|\widetilde{\rho}_q - |\mathbf{\Psi}_0^{(d)}\rangle\langle\mathbf{\Psi}_0^{(d)}|\right\| \lesssim \|h\|\ell^2 d q^{1/2} e^{-a\ell/3} e^{qa^2v^2/2} + e^{-\frac{1}{2}\gamma^2 q}. \tag{3.3.17}$$

Proof. The proof relies on a Duhamel formula:

$$\begin{aligned}\|\widetilde{\rho}_q - |\mathbf{\Psi}_0^{(d)}\rangle\langle\mathbf{\Psi}_0^{(d)}|\| &\leq \|\widetilde{\rho}_q - \rho_q\| + \|\rho_q - |\mathbf{\Psi}_0^{(d)}\rangle\langle\mathbf{\Psi}_0^{(d)}|\|,\\ &\leq \frac{1}{\sqrt{2\pi q}}\int_{\mathbb{R}} \|e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_M(q)+\widetilde{H}_R(q))t} - e^{\mathrm{i}\mathcal{H}^{(d)}t}\|e^{-\frac{t^2}{2q}}\,\mathrm{d}t + e^{-\frac{1}{2}\gamma^2 q},\\ &\lesssim \|h\|\ell^2 dq^{1/2}e^{-a\ell/3}e^{qa^2v^2/2} + e^{-\frac{1}{2}\gamma^2 q},\end{aligned}$$

where we have used Lemma 3.3.11. □

Lemma 3.3.13. *Let $\widetilde{H}_L(q)$ and $\widetilde{H}_R(q)$ be the operators defined in Lemma 3.3.11. Let $\alpha > 0$ and $O_R(q)$ and $O_L(q)$ be the following spectral projections*

$$O_L(q) = \sum_{|\lambda|\leq\alpha} |\Phi_\lambda^{(L)}\rangle\langle\Phi_\lambda^{(L)}|, \quad O_R(q) = \sum_{|\lambda|\leq\alpha} |\Phi_\lambda^{(R)}\rangle\langle\Phi_\lambda^{(R)}|, \tag{3.3.18}$$

where $(\Phi_\lambda^{(L)})$ and $(\Phi_\lambda^{(R)})$ are the normalised eigenvectors of $\widetilde{H}_L(q)$ and $\widetilde{H}_R(q)$. Then we have

$$\|O_R O_L \mathbf{\Psi}_0^{(d)} - \mathbf{\Psi}_0^{(d)}\| \leq \frac{1}{\alpha}\Big(\|\widetilde{H}_L(q) - H_L(q)\| + \|\widetilde{H}_R(q) - H_R(q)\| + \|H_L\mathbf{\Psi}_0^{(d)}\| + \|H_R\mathbf{\Psi}_0^{(d)}\|\Big), \tag{3.3.19}$$

and

$$\|(e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))t} - \mathrm{id})O_L O_R\| \leq 2\alpha|t|. \tag{3.3.20}$$

Proof. We first prove the estimate (3.3.19). Since $O_L(q)$ and $O_R(q)$ commute and are bounded operators by 1, we have

$$\|O_L O_R \mathbf{\Psi}_0^{(d)} - \mathbf{\Psi}_0^{(d)}\| \leq \|O_L\mathbf{\Psi}_0^{(d)} - \mathbf{\Psi}_0^{(d)}\| + \|O_R\mathbf{\Psi}_0^{(d)} - \mathbf{\Psi}_0^{(d)}\|. \tag{3.3.21}$$

We have

$$\begin{aligned}\|O_L\mathbf{\Psi}_0^{(d)} - \mathbf{\Psi}_0^{(d)}\| &\leq \Big\|\int_{|\lambda|\geq\alpha} \mathrm{d}P_\lambda^{\widetilde{H}_L(q)}(\mathbf{\Psi}_0^{(d)})\Big\|\\ &\leq \frac{1}{\alpha}\Big\|\int_{|\lambda|\geq\alpha} \lambda\mathrm{d}P_\lambda^{\widetilde{H}_L(q)}(\mathbf{\Psi}_0^{(d)})\Big\|\\ &\leq \frac{1}{\alpha}\|\widetilde{H}_L(q)\mathbf{\Psi}_0^{(d)}\|\\ &\leq \frac{1}{\alpha}\big(\|\widetilde{H}_L(q) - H_L(q)\| + \|H_L\mathbf{\Psi}_0^{(d)}\|\big).\end{aligned}$$

Estimate (3.3.20) follows from the definition of O_L and O_R. □

A final lemma is needed before completing the proof of Theorem 3.3.6 about the splitting of the evolution $e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_M(q)+\widetilde{H}_R(q))t}$.

Lemma 3.3.14. *With the notation in Lemma 3.3.11, there is a family of operators $\widetilde{H}_M^{(\ell)}(t) \in \mathscr{L}(\mathcal{H}_{j-\ell:j+\ell})$ such that*

$$\left\| e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_M(q)+\widetilde{H}_R(q))t} - \mathcal{T}\exp\Big(\int_0^t \mathrm{id}_{1:j-\ell-1}\otimes\widetilde{H}_M^{(\ell)}(\tau)\otimes\mathrm{id}_{j+\ell+1:d}\,\mathrm{d}\tau\Big)^* e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))t}\right\| \leq t\|h\|\ell^2 d\exp(-a(\ell/3-v|t|)), \quad (3.3.22)$$

where for a family of operators $A(t)$, $\mathcal{T}\exp\big(\int_0^t A(\tau)\,\mathrm{d}\tau\big)$ is the time-ordered exponential.

Proof. We can write

$$e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_M(q)+\widetilde{H}_R(q))t} = e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_M(q)+\widetilde{H}_R(q))t}e^{-\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))t}e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))t}.$$

By differentiating we notice that $e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_M(q)+\widetilde{H}_R(q))t}e^{-\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))t}$ is the solution to

$$\begin{cases} \mathrm{i}U'(t) = U(t)e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))t}H_M e^{-\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))t} \\ U(0) = \mathrm{id}\,. \end{cases}$$

Alternatively, the solution to the equation above can be written

$$e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_M(q)+\widetilde{H}_R(q))t}e^{-\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))t} = \mathcal{T}\exp\Big(\int_0^t e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))\tau}H_M e^{-\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))\tau}\,\mathrm{d}\tau\Big)^*.$$

Using a Lieb-Robinson bound and Corollary 3.3.5, there is a family of operators $\widetilde{H}_M^{(\ell)}(t)$ such that for all $t\in\mathbb{R}$, $\widetilde{H}_M^{(\ell)}(t)\in\mathscr{L}(\mathcal{H}_{j-\ell:j+\ell})$ and

$$\left\| e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))t}H_M e^{-\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))t} - \mathrm{id}_{1:j-\ell-1}\otimes\widetilde{H}_M^{(\ell)}(t)\otimes\mathrm{id}_{j+\ell+1:d}\right\| \leq \|h\|\ell^2 d\exp(-a(\ell/3-v|t|)).$$

It remains to bound the difference between $\mathcal{T}\exp\Big(\int_0^t e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))\tau}H_M e^{-\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))\tau}\,\mathrm{d}\tau\Big)$ and $\mathcal{T}\exp\Big(\int_0^t \mathrm{id}_{1:j-\ell-1}\otimes\widetilde{H}_M^{(\ell)}(\tau)\otimes\mathrm{id}_{j+\ell+1:d}\,\mathrm{d}\tau\Big)$. Recall that for a family of operators $A(t)$, the time-ordered exponential is defined by

$$\mathcal{T}\exp\Big(\int_0^t A(\tau)\,\mathrm{d}\tau\Big) = \lim_{N\to\infty} e^{A(t_N)\Delta t}e^{A(t_{N-1})\Delta t}\cdots e^{A(t_1)\Delta t}, \quad t_k = k\Delta t, \quad \Delta t = \frac{t}{N}.$$

By a Duhamel formula, the difference of the time-ordered exponentials can be bounded by

$$\left\| \mathcal{T}\exp\Big(\int_0^t e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))\tau}H_M e^{-\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))\tau}\,\mathrm{d}\tau\Big) - \mathcal{T}\exp\Big(\int_0^t \mathrm{id}_{1:j-\ell-1}\otimes\widetilde{H}_M^{(\ell)}(\tau)\otimes\mathrm{id}_{j+\ell+1:d}\,\mathrm{d}\tau\Big)\right\| \leq t\|h\|\ell^2 d\exp(-a(\ell/3-v|t|)).$$

This finishes the proof of the lemma. □

We have now all the ingredients to prove Hastings area law 3.3.6.

Proof of Theorem 3.3.6. Let O_L and O_R be the operators defined in Lemma 3.3.13. Then we have

$$|\Psi_0^{(d)}\rangle\langle\Psi_0^{(d)}| = |\Psi_0^{(d)}\rangle\langle\Psi_0^{(d)}|O_LO_R + \frac{1}{\alpha}\mathcal{O}(\|\widetilde{H}_L(q) - H_L(q)\| + \|\widetilde{H}_R(q) - H_R(q)\| + \|H_L\Psi_0^{(d)}\| + \|H_R\Psi_0^{(d)}\|).$$

Thus with Lemma 3.3.10 and Lemma 3.3.11, we obtain

$$|\Psi_0^{(d)}\rangle\langle\Psi_0^{(d)}| = |\Psi_0^{(d)}\rangle\langle\Psi_0^{(d)}|O_LO_R + \frac{1}{\alpha}\mathcal{O}\Big(\gamma J e^{-\frac{1}{2}\gamma^2 q} + \|h\|\ell^2 d q^{1/2} e^{-a\ell/3} e^{qa^2v^2}\Big).$$

Using that O_L and O_R are bounded operators by 1, in combination with Lemma 3.3.12, we get

$$\begin{aligned}|\Psi_0^{(d)}\rangle\langle\Psi_0^{(d)}| &= \frac{1}{\sqrt{2\pi q}}\int_{\mathbb{R}} e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_M(q)+\widetilde{H}_R(q))t} e^{-\frac{t^2}{2q}} O_LO_R \,\mathrm{d}t + \mathcal{O}\Big(\frac{\|h\|\ell^2 d}{\alpha} q^{1/2} e^{-a\ell/3} e^{qa^2v^2} + \frac{\gamma J}{\alpha} e^{-\frac{1}{2}\gamma^2 q}\Big) \\ &= \frac{1}{\sqrt{2\pi q}}\int_{\mathbb{R}} \mathcal{T}\exp\Big(\int_0^t e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))\tau} H_M e^{-\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))\tau}\,\mathrm{d}\tau\Big)^* e^{-\frac{t^2}{2q}} e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))t} O_LO_R \,\mathrm{d}t \\ &\quad + \mathcal{O}\Big(\frac{\|h\|\ell^2 d}{\alpha} q^{1/2} e^{-a\ell/3} e^{qa^2v^2} + \frac{\gamma J}{\alpha} e^{-\frac{1}{2}\gamma^2 q}\Big),\end{aligned}$$

where we have used Lemma 3.3.14. By Lemma 3.3.13, we thus have

$$\begin{aligned}|\Psi_0^{(d)}\rangle\langle\Psi_0^{(d)}| = \frac{1}{\sqrt{2\pi q}}\int_{\mathbb{R}} \mathcal{T}\exp\Big(\int_0^t \mathrm{id}_{1:j-\ell-1}\otimes\widetilde{H}_M^{(\ell)}(\tau)\otimes\mathrm{id}_{j+\ell+1:d}\,\mathrm{d}\tau\Big)^* e^{-\frac{t^2}{2q}} O_LO_R\,\mathrm{d}t \\ + \mathcal{O}\Big(\alpha q^{1/2} + \frac{\|h\|\ell^2 d}{\alpha} q^{1/2} e^{-a\ell/3} e^{qa^2v^2} + \frac{\gamma J}{\alpha} e^{-\frac{1}{2}\gamma^2 q}\Big).\end{aligned}$$

All it remains to do is to set the parameters α and q to prove Theorem 3.3.6. Taking $q = \tilde{q}\ell$ such that $\big(\frac{\gamma^2}{2} + av^2\big)\tilde{q} < \frac{a}{3}$ and $\alpha < e^{-\frac{1}{2}\gamma^2\tilde{q}\ell}$ give (3.3.6). □

3.4 Area laws via AGSP

The main goal of this section is to prove the following Lemma, which is central in the proof of the area law using AGSP.

Lemma 3.4.1 ([AKL16, Theorem 2.3]). *For $\mathcal{J} \subset \{1,\dots,d-1\}$, let $E_0^{\mathcal{J}}$ and $E_0^{(d)}$ be respectively the lowest eigenvalue of $H_{\mathcal{J}} = \sum_{j\in\mathcal{J}} W_j$ and $H^{(d)}$. Let $E_0^{\mathcal{J}}$ be the lowest eigenvalue of $H_{\mathcal{J}}$. Let $\Pi_{[E_0^{\mathcal{J}}+E, E_0^{\mathcal{J}}+E']}$ be the spectral projector of $H_{\mathcal{J}}$ associated to the eigenvalues in $[E_0^{\mathcal{J}}+E, E_0^{\mathcal{J}}+E']$ ($E < E'$). Let $P_{[E_0^{(d)}, E_0^{(d)}+\varepsilon]}$ be the spectral projector of $H^{(d)}$ associated to the eigenvalues in $[E_0^{(d)}, E_0^{(d)}+\varepsilon]$. Then there are constants C and α independent of $E, E', \varepsilon, \mathcal{J}$ such that we have*

$$\|\Pi_{[E_0^{\mathcal{J}}+E, E_0^{\mathcal{J}}+E']} P_{[E_0^{(d)}, E_0^{(d)}+\varepsilon]}\| \le C\exp\Big(-\alpha\big(E - \varepsilon + E_0^{\mathcal{J}} - E_0^{(d)}\big)\Big). \tag{3.4.1}$$

The proof of this estimate relies on the insertion of semigroups $e^{tH_{\mathcal{J}}}$ and $e^{tH^{(d)}}$, with $t > 0$ specified later, between the projectors

$$\begin{aligned}\|\Pi_{[E_0^{\mathcal{J}}+E,E_0^{\mathcal{J}}+E']}P_{[E_0^{(d)},E_0^{(d)}+\varepsilon]}\| &= \|\Pi_{[E_0^{\mathcal{J}}+E,E_0^{\mathcal{J}}+E']}e^{-tH_{\mathcal{J}}}e^{tH_{\mathcal{J}}}e^{-tH^{(d)}}e^{tH^{(d)}}P_{[E_0^{(d)},E_0^{(d)}+\varepsilon]}\| \\ &\leq \|\Pi_{[E_0^{\mathcal{J}}+E,E_0^{\mathcal{J}}+E']}e^{-tH_{\mathcal{J}}}\|\|e^{tH_{\mathcal{J}}}e^{-tH^{(d)}}\|\|e^{tH^{(d)}}P_{[E_0^{(d)},E_0^{(d)}+\varepsilon]}\| \\ &\leq \exp\big(-t(E+E_0^{\mathcal{J}})\big)\|e^{tH_{\mathcal{J}}}e^{-tH^{(d)}}\|\exp\Big(t(E_0^{(d)}+\varepsilon)\Big). \qquad (3.4.2)\end{aligned}$$

It remains to bound $\|e^{tH_{\mathcal{J}}}e^{-tH^{(d)}}\|$. This determines the maximal value t that can be taken.

Let $\overline{\mathcal{J}} = \{j|\exists k \in \mathcal{J}, |j-k| \leq 1$. This is the set of indices which represents the support of the Hamiltonian $H_{\mathcal{J}}$. Let $\overline{\mathcal{J}}^c = \{1,\dots,d\} \setminus \overline{\mathcal{J}}$, $\partial\mathcal{J} = \overline{\mathcal{J}} \setminus \mathcal{J}$. Let $H_{\overline{\mathcal{J}}^c} = \sum_{j\in\overline{\mathcal{J}}^c} W_j$ and $H_{\partial\mathcal{J}} = \sum_{j\in\partial\mathcal{J}} W_j$. Then $H^{(d)} = H_{\mathcal{J}} + H_{\partial\mathcal{J}} + H_{\overline{\mathcal{J}}^c}$ where $H_{\mathcal{J}}$ and $H_{\overline{\mathcal{J}}^c}$ commute, but not $H_{\mathcal{J}}$ and $H_{\partial\mathcal{J}}$, or $H_{\partial\mathcal{J}}$ and $H_{\overline{\mathcal{J}}^c}$. Hence it is not possible to write $e^{tH_{\mathcal{J}}}e^{-tH^{(d)}} = e^{-t(H_{\partial\mathcal{J}}+H_{\overline{\mathcal{J}}^c})}$. There is however a similar but more involved relation that holds.

Lemma 3.4.2 (Dyson expansion [AKL16, Lemma 6.3])**.** *Let X, Y two operators and $t \geq 0$. Then we have*

$$e^{-t(X+Y)} = e^{-tX}\sum_{j=0}^{\infty} G_j(t),$$

where

$$G_j(t) = (-1)^j \int_0^t \mathrm{d}s_1 \int_0^{s_1} \mathrm{d}s_2 \cdots \int_0^{s_{j-1}} \mathrm{d}s_j Y(s_1)\cdots Y(s_j), \qquad (3.4.3)$$

with $Y(s) = e^{sX}Ye^{-sX}$.

With this lemma, we can now prove Lemma 3.4.1.

Proof of Lemma 3.4.1. We are going to apply the Dyson expansion lemma with $X = H_{\mathcal{J}} + H_{\overline{\mathcal{J}}^c}$ and $Y = H_{\partial\mathcal{J}}$. Let $H_{\mathcal{J}\cup\overline{\mathcal{J}}^c} = H_{\mathcal{J}} + H_{\overline{\mathcal{J}}^c}$. We first need to bound $\|e^{sH_{\mathcal{J}\cup\overline{\mathcal{J}}^c}}H_{\partial\mathcal{J}}e^{-sH_{\mathcal{J}\cup\overline{\mathcal{J}}^c}}\|$. For that, we will use the Hadamard expansion [Mil72, Lemma 5.3, pp. 160]

$$e^{sH_{\mathcal{J}\cup\overline{\mathcal{J}}^c}}H_{\partial\mathcal{J}}e^{-sH_{\mathcal{J}\cup\overline{\mathcal{J}}^c}} = H_{\partial\mathcal{J}} + s\big[H_{\mathcal{J}\cup\overline{\mathcal{J}}^c}, H_{\partial\mathcal{J}}\big] + \frac{s^2}{2!}\big[H_{\mathcal{J}\cup\overline{\mathcal{J}}^c}, \big[H_{\mathcal{J}\cup\overline{\mathcal{J}}^c}, H_{\partial\mathcal{J}}\big]\big] + \dots$$

Because of the nearest neighbour interaction structure of the Hamiltonian, most of the terms in the iterated commutator vanish. Let $k \in \partial\mathcal{J}$. By linearity it is enough to consider the iterated commutator of $\big[H_{\mathcal{J}\cup\overline{\mathcal{J}}^c}, \dots \big[H_{\mathcal{J}\cup\overline{\mathcal{J}}^c}, W_k\big]\dots\big]$. Denote $K_n = \underbrace{\big[H_{\mathcal{J}\cup\overline{\mathcal{J}}^c}, \dots \big[H_{\mathcal{J}\cup\overline{\mathcal{J}}^c}}_{n \text{ times}}, W_k\big]\dots\big]$. Then the only non vanishing terms in the iterated commutator are terms of the form $\prod_{j=1}^n W_{i_j}$ where $\{i_1,\dots,i_n\}$ is -up to reordering- a list of at most n consecutive integers including k. Hence the number of non vanishing terms when expanding the iterated commutator is bounded

by $6^n n!$ because $[A,B] = AB - BA$ and W_j has common support with W_{j-1}, W_j, W_{j+1}. Thus we have

$$\|K_n\| \leq 6^n \|W\|^{n+1} n!,$$

hence

$$\|e^{sH_{\mathcal{J}\cup\overline{\mathcal{J}}^c} H_{\partial\mathcal{J}} e^{-sH_{\mathcal{J}\cup\overline{\mathcal{J}}^c}}\| \leq \sum_{n=0}^{\infty} |\partial\mathcal{J}| 6^n \|W\|^{n+1} s^n \leq \frac{|\partial\mathcal{J}|\|W\|}{1-6s\|W\|}, \tag{3.4.4}$$

for $0 \leq s < \frac{1}{6\|W\|}$.

We can now bound $\|G_j(t)\|$ in (3.4.3) with $X = H_{\mathcal{J}\cup\overline{\mathcal{J}}^c}$ and $Y = H_{\partial\mathcal{J}}$. We have for $0 \leq t < \frac{1}{6\|W\|}$

$$\begin{aligned}
\|G_j(t)\| &= \Big\| \int_0^t \mathrm{d}s_1 \int_0^{s_1} \mathrm{d}s_2 \cdots \int_0^{s_{j-1}} \mathrm{d}s_j H_{\partial\mathcal{J}}(s_1) \cdots H_{\partial\mathcal{J}}(s_j) \Big\| \\
&\leq \int_0^t \mathrm{d}s_1 \int_0^{s_1} \mathrm{d}s_2 \cdots \int_0^{s_{j-1}} \mathrm{d}s_j \, \|H_{\partial\mathcal{J}}(s_1)\| \ldots \|H_{\partial\mathcal{J}}(s_j)\| \\
&\leq \frac{(|\partial\mathcal{J}|\|W\|t)^j}{j!(1-6\|W\|t)^j}.
\end{aligned}$$

Thus we have

$$\Big\| \sum_{j=0}^{\infty} G_j(t) \Big\| \leq \sum_{j=0}^{\infty} \frac{(|\partial\mathcal{J}|\|W\|t)^j}{j!(1-6\|W\|t)^j} = \exp\left(\frac{|\partial\mathcal{J}|\|W\|}{1-6\|W\|t} t \right). \tag{3.4.5}$$

For any $0 < t < \frac{1}{6\|W\|}$, we have

$$\begin{aligned}
\left\| e^{tH_{\mathcal{J}}} e^{-tH^{(d)}} \right\| &\leq \left\| e^{tH_{\mathcal{J}}} e^{-tH_{\mathcal{J}\cup\overline{\mathcal{J}}^c}} \sum_{j=0}^{\infty} G_j(t) \right\| \\
&\leq \|e^{-tH_{\overline{\mathcal{J}}^c}}\| \Big\| \sum_{j=0}^{\infty} G_j(t) \Big\| \\
&\leq \exp\left(\frac{|\partial\mathcal{J}|\|W\|}{1-6\|W\|t} t \right),
\end{aligned}$$

where we have used that $H_{\mathcal{J}}$ and $H_{\overline{\mathcal{J}}^c}$ commute and $H_{\overline{\mathcal{J}}^c} \geq 0$.

Inserting the last estimate in Eq. (3.4.2) finishes the proof of the lemma. □

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