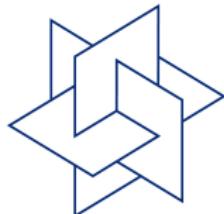


Density Matrix Renormalization Group Algorithm - Optimization in TT-format

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Mathematics for key technologies



Density Matrix Renormalisation Group (DMRG)

DMRG algorithm is prominent algorithm to treat many body quantum systems (<http://en.wikipedia.org/wiki/DMRG>)

- ▶ S. White (1991) spin chains
- ▶ S. White & Jourdan (1999) quantum chemistry
- ▶ G. Chan & Head-Gordon (2002) electronic structure computation
- ▶ ... O. Legeza et al. or M. Reiher et al.

DMRG provides an (approximate) FCI algorithm in polynomial complexity

dynamical correlation (short range - ee-cusp)	statical or strong correlation (multi-configurational)
Coupled Cluster (CCSD-)	CASPT-MRSCF - DMRG

Setting - Tensors

$$V_\nu := \mathbb{R}^n .$$

$\mathcal{H}_d = \mathcal{H} := \bigotimes_{\nu=1}^d V_\nu$ d -fold tensor product Hilbert space,

$$\mathcal{H} \simeq \{(x_1, \dots, x_d) \mapsto U(x_1, \dots, x_d) \in \mathbb{R} : x_i = 1, \dots, n\} .$$

The function $U \in \mathcal{H}$ will be called an **order d -tensor**.

Here x_1, \dots, x_d will be called **variables** or **indices**.

$$\mathbf{k} \mapsto u(k_1, \dots, k_d) = (u_{k_1, \dots, k_d}) = \mathbf{u} , \quad k_i = 1 \dots, n .$$

Operators (matrization)

$$\mathbf{A} =: (a_k^l)_{k,l} , \quad \mathbf{A} = (A_{x_1, \dots, x_d}^{k_1, \dots, k_l}) := (a_{x_1, \dots, x_d, k_1, \dots, k_l}) .$$

TT - Tensors

$$\mathbf{u}^{k_\nu} = {}^\nu \mathbf{u}^{k_\nu} = (u_{x_\nu, k_{\nu-1}, k_\nu}) .$$

$$\sum_{\mathbf{k} < j}^{\mathbf{r}} := \sum_{k_0=1}^{r_1} \dots \sum_{k_{j-1}}^{r_{j-1}} , \quad \sum_{\mathbf{k} > j}^{\mathbf{r}} := \sum_{k_{j+1}}^{r_{j+1}} \dots \sum_{k_d}^{r_d} .$$

If $k_0 := 1, k_d := 1$ (single index), a tensor \mathbf{U} in the TT-format is

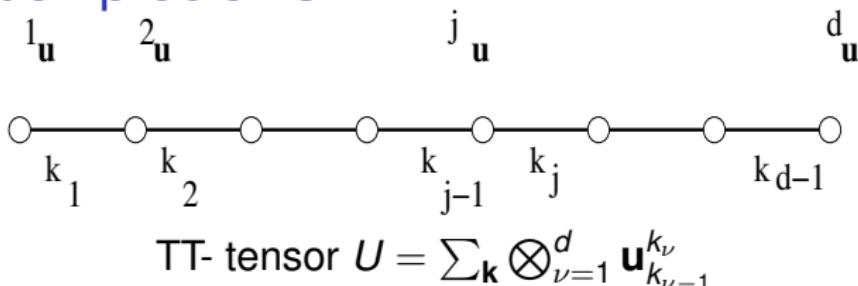
$$\mathbf{U} = \sum_{k_0=1}^{r_1} \dots \sum_{k_d}^{r_d} \bigotimes_{\nu=1}^d {}^\nu \mathbf{u}_{k_{\nu-1}}^{k_\nu} = \sum_{\mathbf{k} \leq d}^{\mathbf{r}} \bigotimes_{\nu=1}^d \mathbf{u}_{k_{\nu-1}}^{k_\nu} \in \mathcal{T}\mathcal{T}^{\mathbf{r}} .$$

$\mathbf{u}^{k_\nu} = (u_{x_\nu, k_{\nu-1}}^{k_\nu})_{x_\nu, k_{\nu-1}}$ $1 \leq \nu < d$, could be orthonormalized.

For operators $\mathbf{A} : \mathcal{H}^d \rightarrow \mathcal{H}^d$, $\mathbf{A} : \mathcal{H} \rightarrow \mathcal{H}$:

$$\mathbf{a}_{k_{\nu-1}}^{k_\nu} = ((a_{x_\nu}^{y_\nu})_{k_{\nu-1}}^{k_\nu}) = (a_{x_\nu, k_{\nu-1}}^{y_\nu, k_\nu})_{x_\nu, y_\nu}$$

Optimization problems



Tensor optimization

Approximate $W \in \mathcal{H}$: by a tensor of (canonial) rank \mathbf{r}
Linear elliptic equations

$$U = \operatorname{argmin} \{ F(V) = \frac{1}{2} \langle AV, V \rangle - \langle B, V \rangle : V \in \mathcal{T}\mathcal{T}^* \} .$$

eigenvalue problems

$$U = \operatorname{argmin} \{ F(V) = \frac{1}{2} \langle AV, V \rangle - \langle V, V \rangle = 1 : V \in \mathcal{T}\mathcal{T}^* \} .$$

→ for general optimization problems $F : \mathcal{H}_d \rightarrow \mathbb{R}$ Espig & Hackbusch & Rohwedder

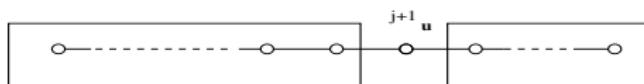
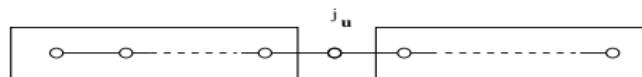
Optimization by relaxation in TT format

Relaxation (see e.g. Gauss-Seidel, ALS):

For $j = 1, \dots, d$:

1. fix all tensors ${}^\nu \mathbf{u}_{k_{\nu-1}}^{k_\nu}$, $\nu \in \{1, \dots, d\} \setminus \{j\}$, except the index j .
2. Optimize $\mathbf{u}_{k_{j-1}}^{k_j} := {}^j \mathbf{u}_{k_{j-1}}^{k_j}$.

Repeat the relaxation procedure (in the opposite direction.)



Relaxation scheme $\mathbf{u}_{k_{j-1}}^{k_\nu}$

This is NOT exactly the DMRG algorithm!

Relaxation in TT format

$$\mathbf{U} = \sum_{k_{j-1}, k_j} \ell^{k_{j-1}} \otimes \mathbf{u}_{k_{j-1}}^{k_j} \otimes \mathbf{r}_{k_j},$$

where

$$\ell^{k_{j-1}} := \sum_{\mathbf{k} < j} \bigotimes_{\nu=1}^{j-1} \mathbf{u}_{k_{\nu-1}}^{k_\nu}, \quad \mathbf{r}_{k_j} := \sum_{\mathbf{k} < j} \bigotimes_{\nu=j+1}^d \mathbf{u}_{k_{\nu-1}}^{k_\nu}.$$

operators in TT format

$$\mathbf{A} = \sum_{l_{j-1}, l_j} \mathbf{A}_L^{l_{j-1}} \otimes \mathbf{a}_{l_{j-1}}^{l_j} \otimes \mathbf{A}_{Rl_j}$$

$$\mathbf{A}_L^{l_{j-1}} = \sum_{\mathbf{l} < j} \bigotimes_{\nu=1}^{j-1} \mathbf{a}_{l_{\nu-1}}^{l_\nu}, \quad \mathbf{A}_{Rl_j} = \sum_{\mathbf{l} > j} \bigotimes_{\nu=j+1}^d \mathbf{a}_{l_{\nu-1}}^{l_\nu}.$$

Stationary condition

For simplicity of representation, let us assume in the sequel:

Rank $\mathbf{A} = 1$, i.e. $\mathbf{A} = \bigotimes_{\nu=1}^d \mathbf{a}_\nu$.

For fixed j , the stationary condition is

$$\sum_{k'_{j-1}, k'_j} \langle \ell^{k_{j-1}}, \mathbf{A}_L \ell^{k'_{j-1}} \rangle (\mathbf{a} \mathbf{u}_{k_j}^{k_{j-1}}) \langle \mathbf{r}_{k_j}, \mathbf{A}_R \mathbf{r}_{k'_j} \rangle = \mathbf{b}_{k_{j-1}}^{k_j} \in \mathbb{R}^n , \quad *$$

$$\forall k_{j-1} = 1, \dots, r_{j-1} , \quad k_j = 1, \dots, r_j , \quad \mathbb{R}^n = \text{span}\{\mathbf{e}_i\} ,$$

where

$$\langle \mathbf{e}_i, \mathbf{b}_{k_{j-1}} k_j \rangle := \langle \mathbf{B}, \ell^{k_{j-1}} \otimes \mathbf{e}_i \otimes \mathbf{r}_{k_j} \rangle , \quad i = 1, \dots, n .$$

* Rank $\mathbf{A} = 1$

Stationary condition

Defining the tensors

$$\mathbf{G} := ((\mathbf{g})_{k_{j-1}}^{k'_{j-1}}) = \langle \ell^{k_{j-1}}, \mathbf{A}_L \ell^{k'_{j-1}} \rangle ,$$

$$\mathbf{H} := ((\mathbf{h})_{k_j}^{k'_j}) = \langle \mathbf{r}_{k_j}, \mathbf{A}_R \mathbf{r}_{k'_j} \rangle ,$$

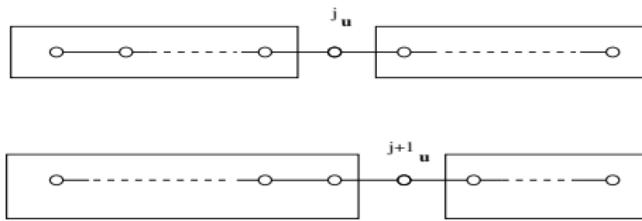
and let $\mathbf{u} := (u_{k_{j-1}, x_j, k_j})$, $\mathbf{b} := (b_{k_{j-1}, x_j, k_j})$

For fixed j , the stationary condition is

$$\tilde{\mathbf{A}} \mathbf{u} = (\mathbf{G} \otimes \mathbf{a} \otimes \mathbf{H}) \mathbf{u} = \mathbf{b} . \quad *$$

* Rank $\mathbf{A} = 1$

Update $j \rightarrow j + 1$



$j \rightarrow j + 1$: update ${}^j \mathbf{G} \rightarrow {}^{j+1} \mathbf{G} =: \mathbf{G}$,

$$g_{k_j}^{k'_j} = \sum_{x_j, y_j=1}^n \sum_{k_{j-1}, k'_{j-1}=0}^{r_{j-1}} u_{x_j, k_{j-1}}^{k_j} g_{k_{j-1}}^{k'_{j-1}} a_{x_j}^{y_j} u_{x_j, k'_{j-1}}^{k'_j}. \quad *$$

shortly

$${}^{j+1} \mathbf{G} := \mathbf{u}^T ({}^j \mathbf{G} \otimes \mathbf{a}) \mathbf{u}, \quad (u_{x_j, k_{j-1}}^{k_j}) := (u_{x_j, k_{j-1}}^{k_j}) \quad *$$

For $\nu = 1, \dots, d$, ${}^\nu \mathbf{H}$ are computed once and stored.

* Rank $\mathbf{A} = 1$

Eigenvalue problem

$$\mathbf{A} = \mathbf{I} \Rightarrow \tilde{\mathbf{M}} := (\mathbf{P} \otimes \mathbf{I} \otimes \mathbf{Q})$$

where

$$\mathbf{P} = ((\mathbf{p})_{k_{j-1}}^{k'_{j-1}}) = \langle \ell^{k_{j-1}}, \ell^{k'_{j-1}} \rangle, \quad \mathbf{Q} := ((\mathbf{q})_{k_j}^{k'_j}) = \langle \mathbf{r}_{k_j}, \mathbf{r}_{k'_j} \rangle.$$

If ℓ^{k_ν} and/or \mathbf{r}^{k_ν} are orthonormal, then $\mathbf{P} = \mathbf{I}$, $\mathbf{Q} = \mathbf{I}$.

(EVP): Generalized eigenvalue problem

$$\tilde{\mathbf{A}}\mathbf{u} := (\mathbf{G} \otimes \mathbf{a} \otimes \mathbf{H})\mathbf{u} = \lambda \tilde{\mathbf{M}}\mathbf{u} = \lambda (\mathbf{P} \otimes \mathbf{I} \otimes \mathbf{Q})\mathbf{u}.$$

*

* Rank $\mathbf{A} = 1$

Stationary condition -general case

$$\sum_{l_{j-1}, l_j} \sum_{k'_{j-1}, k'_j} \langle \ell^{k_{j-1}}, \mathbf{A}_L^{l_{j-1}} \ell^{k'_{j-1}} \rangle (\mathbf{a}_{l_{j-1}}^{l_j} \mathbf{u}_{k'_j}^{k_{j-1}}) \langle \mathbf{r}_{k_j}, \mathbf{A}_{Rl_j} \mathbf{r}_{k'_j} \rangle = \mathbf{b}_{k_{j-1}}^{k_j} \in \mathbb{R}^n,$$

$$\forall k_{j-1} = 1, \dots, r_{j-1}, \quad k_j = 1, \dots, r_j, \quad \mathbb{R}^n = \text{span}\{\mathbf{e}_i\},$$

where

$$\langle \mathbf{e}_i, \mathbf{b}_{k_{j-1}} k_j \rangle := \langle \mathbf{B}, \ell^{k_{j-1}} \otimes \mathbf{e}_i \otimes \mathbf{r}_{k_j} \rangle, \quad i = 1, \dots, n.$$

Defining the tensors

$$\mathbf{G} := ((\mathbf{g}_{l_{j-1}})^{k'_{j-1}}_{k_{j-1}}) = \langle \ell^{k_{j-1}}, \mathbf{A}_L^{l_{j-1}} \ell^{k'_{j-1}} \rangle,$$

$$\mathbf{H} := ((\mathbf{h}_{l_j})^{k'_j}_{k_j}) = \langle \mathbf{r}_{k_j}, \mathbf{A}_{Rl_j} \mathbf{r}_{k'_j} \rangle,$$

the stationary condition is equivalent to the linear equation

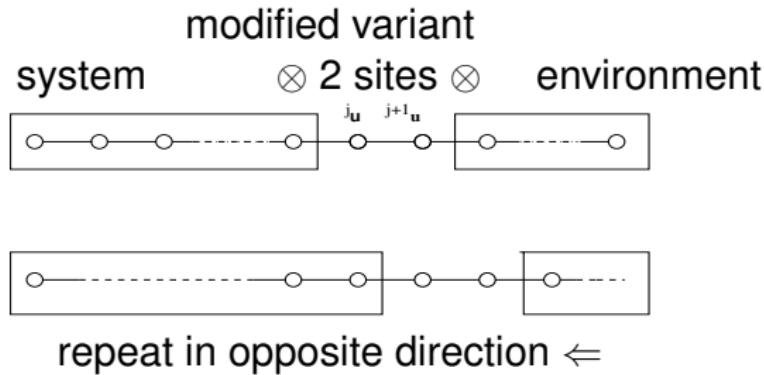
$$\boxed{\sum_{l_{j-1}, l_j} (\mathbf{g}_{l_{j-1}})^{k'_{j-1}}_{k_{j-1}} (\mathbf{a}_{l_{j-1}}^{l_j} \mathbf{u}_{k'_j}^{k_{j-1}}) (\mathbf{h}_{l_j})^{k'_j}_{k_j} = \mathbf{b}_{k_{j-1}}^{k_j} \quad \forall k_{j-1}, k_j.}$$

A modified relaxation algorithm

Disadvantage of simple relaxation:

1. $\mathbf{u}^{k_{j+1}}$ not orthogonal,
2. $\mathbf{r} = (r_1, \dots, r_d)$ is fixed ...

Idea: optimize $(\mathbf{w}_{x_j, x_{j+1}})_{k_{j-1}}^{k_{j+1}} \approx \sum_{k_j}^{r_j} (\mathbf{u}_{x_j})_{k_{j-1}}^{k_j} (\mathbf{v}_{x_{j+1}})_{k_j}^{k_{j+1}}$.



* Rank $\mathbf{A} = 1$

A modified relaxation algorithm

n small, e.g. $n = 2, 4$ etc. (complexity $\mathcal{O}(n) \rightarrow \mathcal{O}(n^2)$)

Modified - Relaxation:

For $j = 1, \dots, d$:

1. fix all tensors $\mathbf{u}_{k_{\nu-1}}^{k_\nu}$, $\nu \in \{1, \dots, d\} \setminus \{j, j+1\}$, except $j, j+1$.
2. Optimize $\mathbf{w}_{k_{j-1}}^{k_{j+1}} := (\mathbf{w}_{x_j, x_{j+1}})_{k_{j-1}}^{k_{j+1}}$.
3. Decimation by SVD:

$$(\mathbf{w}_{x_j, x_{j+1}})_{k_{j-1}}^{k_{j+1}} \approx \sum_{k_j}^{r_j} (\mathbf{u}_{x_j})_{k_{j-1}}^{k_j} (\mathbf{v}_{x_{j+1}})_{k_j}^{k_{j+1}}.$$

4. update $\mathbf{G} = {}^{j+1}\mathbf{G}$, (since $\mathbf{P} = \mathbf{I}$)

$${}^{j+1}\mathbf{G} := \mathbf{u}^T ({}^j\mathbf{G} \otimes \mathbf{a}) \mathbf{u}, \quad (u_{x_j, k_{j-1}}^{k_j}) := (u_{x_j, k_{j-1}}^{k_j})^*$$

Repeat the relaxation procedure in the opposite direction
 $\Rightarrow \mathbf{Q} = \mathbf{I}$.

* Rank $\mathbf{A} = 1$

Conclusions

1. \mathbf{u}^k are ortho-normal $\Rightarrow \mathbf{P} = \mathbf{I}, \mathbf{Q} = \mathbf{I}$,
2. the ranks could be adapted by the SVD
3. SVD provides indication about the error

Complexity:

TT rank: $R; = \max\{r_\nu\}$

TT rank of \mathbf{A} : R_A ,
canonical rank of \mathbf{A} : M_A

Storage : $\mathcal{O}(R^2 R_A d) + \mathcal{O}(n^2 R^2)$, $\mathcal{O}(R^2 M_A d) + \mathcal{O}(n^2 R^2)$

Computing time: $\mathcal{O}(n^2 R^3 R_A^2 d) + \mathcal{O}(n^2 R^3)$, $\mathcal{O}(n^2 R^3 M_A d) + \mathcal{O}(n^2 R^3 d)$

Fock space

Let $\Psi_\mu := \Psi_{SL}[\varphi_{k_1}, \dots, \varphi_{k_N}] = \Psi[k_1, \dots, k_N]$ basis Slater det.

Labeling of indices $\mu \in \mathcal{I}$ by an binary string of length d

$$\text{e.g.: } \mu = (0, 0, 1, 1, 0, \dots) =: \sum_{i=1}^d \mu_i 2^{d-i+1}, \quad \mu_i = 0, 1,$$

- $\mu_i = 1$ means φ_i is (occupied) in $\Psi[\dots]$.
- $\mu_i = 0$ means φ_i is absend (not occupied) in $\Psi[\dots]$.

(discrete) Fock space $\bigoplus_{\mu} \mathcal{V}_{FCI}^N$ is of $\dim \mathcal{F} = 2^d$,

$$\mathcal{F} := \bigoplus_{N=0}^d \mathcal{V}_{FCI}^N = \{\Psi : \Psi = \sum_{\mu} c_{\mu} \Psi_{\mu}\}$$

$$\mathcal{F} \simeq \{\mathbf{c} : \mu \mapsto \mathbf{c}(\mu_1, \dots, \mu_d) = c_{\mu}, \quad \mu_i = 0, 1, \quad i = 1, \dots, d\} = \bigotimes_{i=1}^d \mathbb{R}^2$$

configuration space

$$d \rightarrow \infty : \bigotimes_{j=1}^N \bigoplus_{k=1}^{\infty} \text{span}\{\varphi_k\} \leftrightarrow \bigotimes_{j=1}^{\infty} \mathbb{R}^2$$

work in progress Holtz & S.

Discrete annihilation and creation operators

$$A := \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, A^T = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

Let us observe

$$\begin{aligned} B := A^T A &= \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, AA^T = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \\ \Rightarrow A^2 &= 0, AA^T + A^T A = I, \end{aligned}$$

In order to obtain the correct phase factor, we define

$$S := \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix},$$

and the discrete **annihilation operator**

$$a_p \simeq \mathbf{A}_p := I \otimes \dots \otimes A_{(p)} \otimes S \otimes \dots \otimes S$$

where $A_{(p)}$ means that A appears on the p -th position in the product.

Schrödinger operator

The creation operator

$$a_p^\dagger \simeq \mathbf{A}_p^T := I \otimes \dots \otimes A_{(p)}^T \otimes S \otimes \dots \otimes S$$

We have the one-to-one correspondence

$$a_p^\dagger \simeq \mathbf{A}_p^T , \quad a_p \simeq \mathbf{A}_p .$$

Single particle operator, e.g. Fock operator

$$F := \sum_{r,p} f_p^q a_q^\dagger a_p \simeq \sum_{p,q} f_q^p \mathbf{A}_p^T \mathbf{A}_p .$$

Schrödinger-Hamilton operator

$$H = \sum_{p,q} h_p^q a_q^\dagger a_p + \sum_{p,q,r,s} g_{r,s}^{p,q} a_r^\dagger a_s^\dagger a_q a_p \simeq$$

$$\mathbf{H} = \sum_{p,q=1}^d h_p^q \mathbf{A}_p^T \mathbf{A}_q + \sum_{p,q,r,s=1}^d g_{r,s}^{p,q} \mathbf{A}_r^T \mathbf{A}_s^T \mathbf{A}_p \mathbf{A}_q .$$

Particle number operator and Schrödinger eqn.

$$P := \sum_{p=1}^d a_p^\dagger a_p, \quad \simeq \quad \mathbf{P} := \sum_{p=1}^d \mathbf{A}_p^T \mathbf{A}_p.$$

The space of N -particle states is given by

$$\mathcal{V}_{FCI}^N := \{\Psi \in \mathcal{F} : P\Psi = N\Psi\} . \simeq \mathcal{V}^N := \{\mathbf{c} \in \bigotimes_{i=1}^d \mathbb{R}^2 : \mathbf{P}\mathbf{c} = N\mathbf{c}\} .$$

Variational formulation of the Schrödinger equation

$$\mathbf{c} = (c(\mu)) = \operatorname{argmin}\{\langle \mathbf{H}\mathbf{c}, \mathbf{c} \rangle : \langle \mathbf{c}, \mathbf{c} \rangle = 1, \mathbf{P}\mathbf{c} = N\mathbf{c}\} .$$

Example

Let $\mathbb{R}^2 = \operatorname{span}\{e^0, e^1\}$, a single Slater determinant, e.g HF determinant, is rank 1 in $\bigotimes_{i=1}^d \mathbb{R}^2$, e.g.

$$\Psi[1, \dots, N] \simeq e_{(0)}^1 \otimes \dots \otimes e_{(N)}^1 \otimes e_{(N+1)}^0 \otimes \dots \otimes e_{(d)}^0 \in \mathcal{V}^N .$$

DMRG

n small, e.g. $n = 2, 4$ etc. (complexity $\mathcal{O}(n) \rightarrow \mathcal{O}(n^2)$)

DMRG - Relaxation:

For $j = 1, \dots, d$:

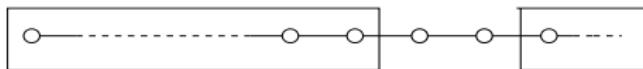
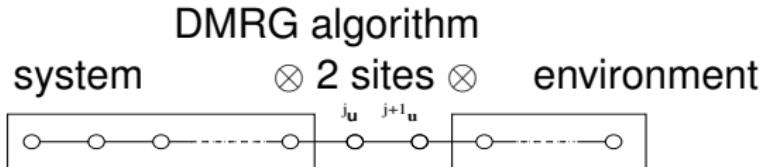
1. fix all tensors $\mathbf{u}_{k_{\nu-1}}^{k_\nu}$, $\nu \in \{1, \dots, d\} \setminus \{j, j+1\}$, except $j, j+1$.
2. Optimize $\mathbf{w}_{k_{j-1}}^{k_{j+1}} := (\mathbf{w}_{x_j, x_{j+1}})_{k_{j-1}}^{k_{j+1}}$.
3. Decimation by SVD: $(\mathbf{w}_{x_j, x_{j+1}})_{k_{j-1}}^{k_{j+1}} \approx \sum_{k_j}^{r_j} (\mathbf{u}_{x_j})_{k_{j-1}}^{k_j} (\mathbf{v}_{x_{j+1}})_{k_j}^{k_{j+1}}$.
4. update $\mathbf{G} = {}^{j+1}\mathbf{G}$, (since $\mathbf{P} = \mathbf{I}$)

$${}^{j+1}\mathbf{G} := \mathbf{u}^T ({}^j\mathbf{G} \otimes \mathbf{a}) \mathbf{u} , \quad *$$

Repeat the relaxation procedure in opposite direction ($\mathbf{Q} = \mathbf{I}$).

* Rank $\mathbf{A} = 1$

DMRG for the eigenvalue problem



Super system $\tilde{\mathbf{A}}\mathbf{w} := (\mathbf{G} \otimes^j \mathbf{a} \otimes^{j+1} \mathbf{a} \otimes \mathbf{H})\mathbf{w} = \lambda \mathbf{l}\mathbf{w}$ *

\Rightarrow

Decimation (SVD) \Rightarrow update
repeat in opposite direction \Leftarrow

* Rank $\mathbf{A} = 1$

DMRG for the eigenvalue problem

Warm up sweep: ${}^J\mathbf{P} = \mathbf{I}$, ${}^J\mathbf{Q} = \mathbf{I}$ $\forall j$ and ${}^J\mathbf{H}$, ${}^J\mathbf{G}$ are computed.

For $j = 1, \dots, d$:

1. Optimize $\mathbf{w}_{k_{j-1}}^{k_{j+1}} := (\mathbf{w}_{x_j, x_{j+1}})_{k_{j-1}}^{k_{j+1}}$, super-block Hamiltonian $\widetilde{\mathbf{A}}$: with particle number N and z-spin m_z

$$\widetilde{\mathbf{A}}\mathbf{w} := (\mathbf{G} \otimes {}^j\mathbf{a} \otimes {}^{j+1}\mathbf{a} \otimes \mathbf{H})\mathbf{w} = \lambda \mathbf{I}\mathbf{w}. \quad *$$

2. Decimation by SVD: $(\mathbf{w}_{x_j, x_{j+1}})_{k_{j-1}}^{k_{j+1}} \approx \sum_{k_j}^{r_j} (\mathbf{u}_{x_j})_{k_{j-1}}^{k_j} (\mathbf{v}_{x_{j+1}})_{k_j}^{k_{j+1}}$,
e.g. by diagonalizing density matrix

$$\mathbf{D}\mathbf{u} := (\mathbf{w}^T \mathbf{w})\mathbf{u} = \mu \mathbf{u},$$

3. update $\mathbf{G} = {}^{j+1}\mathbf{G}$, (since $\mathbf{P} = \mathbf{I}$)

$$\mathbf{G} \leftarrow \mathbf{u}^T (\mathbf{G} \otimes {}^j\mathbf{a}) \mathbf{u}. \quad *$$

Repeat the relaxation procedure in the opposite direction
 $j + 1 \rightarrow j \Rightarrow$ if convergence $\Rightarrow \lambda_i = E_i$, $i = 0, \dots$

* Rank $\mathbf{A} = 1$

Quantum chemistry

1. For $\lambda_i = E_i$, the tensor \mathbf{u} is only used for updating \mathbf{G} (the full tensor has never been considered)
2. \mathbf{u}^k are ortho-normal $\Rightarrow \mathbf{P} = \mathbf{I}, \mathbf{Q} = \mathbf{I},$
3. additional constraint conditions, like for fixed quantum numbers e.g. N could be applied
4. the ranks could be adapted by the SVD
5. SVD provides indication about the error

In quantum chemistry: $n = 2$ ($n = 4$),
 $M_A = \mathcal{O}(d^2)$ ($M_A = \mathcal{O}(d^3)$) $R_A = \mathcal{O}(d^{??})$,

For a fixed N electron system and increasing d

storage: $\mathcal{O}(R^2 d^3)$, computing time: $\mathcal{O}(R^3 d^3)$.

$R \approx \mathcal{O}(d - d^2)???$ (100 – 6000 ...) measure for entanglement