Alternating linear scheme ALS and MALS and the DMRG algrithm

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John von Neumann Lecture – TU Munich, 2012

Setting - Tensors

$$V_\nu := \mathbb{R}^n \ , \ \ \mathcal{H}_d = \mathcal{H} := \bigotimes_{\nu=1}^{d} V_\nu$$ d-fold tensor product Hilbert-s.,

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

The function $U \in \mathcal{H}$ will be called an order d-tensor.
For notational simplicity, we often consider $n_i = n$. Here
$x_1, \ldots, x_d \in \{1, \ldots, n\}$ will be called variables or indices.

$$\mathbf{k} \mapsto U(k_1, \ldots, k_d) = (U_{k_1,\ldots,k_d}) \ , \ \ k_i = 1 \ldots, n_i \ .$$

Or in index (vectorial) notation

$$\mathbf{U} = \left(U_{k_1,\ldots,k_d}\right)_{k_i=0, 1 \leq i \leq d}^{n_i}$$

$$\dim \mathcal{H} = n^d$$ curse of dimensions!!!

E.g. wave function $\Psi(\mathbf{r}_1, s_1, \ldots, \mathbf{r}_N, s_N)$

TT - Tensors - Matrix product representation

Noteable special case of HT:

TT format (Oseledets & Tyrtyshnikov, 2009)

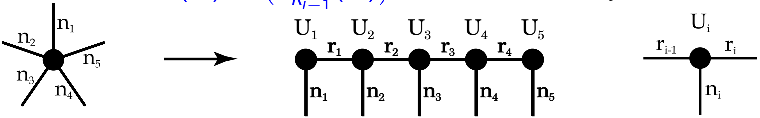
(matrix product states (MPS), Östlund & ROmmer (1995), Vidal 2003, Schöllwock et al.)

Tensor U in the TT-representation written as matrix product

$$U(\mathbf{x}) = \mathbf{U}_1(x_1)\cdots\mathbf{U}_\nu(x_\nu)\cdots\mathbf{U}_d(x_d)$$

$$= \sum_{k_1=1}^{r_1} .. \sum_{k_{d-1}=1}^{r_{d-1}} U_1(x_1,k_1)U_2(k_1,x_1,k_2)...U_{d-1}(k_{d-2}x_{d-1},k_{d-1})U_d(k_{d-1},x_d,k_d)$$

with matrices $\mathbf{U}_i(x_i) = \left(u^{k_i}_{k_{i-1}}(x_i)\right) \in \mathbb{R}^{r_{i-1}\times r_i}$, $r_0 = r_d := 1$



- component tensors $U_i(k_{i-1},x_i,k_i) \in \mathbb{R}^{r_{i-1}\times n_i\times r_i}$
- Component functions $\mathbf{U}_i : x_i \mapsto \mathbf{U}_i(x_i) \in \mathbb{R}^{r_{i-1}\times r_i}$

Definitions: TT rank, separation rank

$\mathbf{U}_i(x_i) : \{1, \ldots, n_i\} \to \mathbb{R}^{r_{i-1} \times r_i}$,

$$\text{left matricisation } \mathbf{L}\big(\mathbf{U}_i(x_i)\big) := \big[U^{k_i}_{k_{i-1}, x_i}\big]$$

left orthogonal

$$\mathbf{L}\big(\mathbf{U}_i(x_i)\big)^T \mathbf{L}\big(\mathbf{U}_i(x_i)\big) = \sum_{k_{i-1}, x_i} \mathbf{U}_i(k_{i-1}, x_i, k_i')\mathbf{U}_i(k_{i-1}, x_i, k_i) = \delta_{k_i', k_i}$$

$\mathbf{U}_i(x_i) : \{1, \ldots, n_i\} \to \mathbb{R}^{r_{i-1} \times r_i}$ satisfies full rank condition iff

$$\boxed{\text{rank } \mathbf{L}\big(\mathbf{U}_i(x_i)\big) \;=\; r_i \;=\; \text{rank } \mathbf{R}\big(\mathbf{U}_{i+1}(x_{i+1})\big).}$$

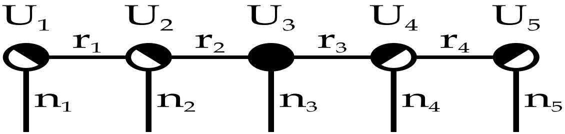
If all component functions $\mathbf{U}_i(x_i)$ of a TT decomposition

$$U(\mathbf{x}) \;=\; \mathbf{U}_1(x_1)\mathbf{U}_2(x_2) \cdot \ldots \cdot \mathbf{U}_{d-1}(x_{d-1})\mathbf{U}_d(x_d)$$

satisfy the full rank condition, it has TT rank $\underline{r} = (r_1, \ldots, r_{d-1})$.
This is equal to the *i-th seperation rank* s_i of U:

$$\boxed{\text{Rank of } \mathbf{A}_i = U^{x_{i+1}, \ldots, x_d}_{x_1, \ldots, x_i} = s_i = r_i\ .}$$

Nonlinear Galerkin Ritz formulation



TT- tensor $U = \sum_{\mathbf{k}} \bigotimes_{\nu=1}^{d} \mathbf{u}_{k_{\nu-1}}^{k_\nu}$

Tensor optimization

Approximation of $W \in \mathcal{H}$: by a tensor of (canonial) rank **r**

$$U = \text{argmin}\left\{F(V) = \frac{1}{2}\langle V - W, V - W\rangle : V \in \mathbb{T}_{\mathbf{r}}\right\} .$$

Linear elliptic equations

$$U = \text{argmin}\left\{F(V) = \frac{1}{2}\langle AV, V\rangle - \langle B, V\rangle : V \in \mathbb{T}_{\mathbf{r}}\right\} .$$

eigenvalue problems

$$U = \text{argmin}\left\{F(V) = \langle AV, V\rangle : \langle V, V\rangle = 1 : V \in \mathbb{T}_{\mathbf{r}}\right\} .$$

Existence

Setting includes elliptic PDE's in high dimensions.
Weak closedness (Hackbusch & Falco (2010))

$$\mathbb{T}_{\leq \mathbf{r}} = \bigcup_{s_i \leq r_i : 1 \leq i < d} \mathbb{T}_{\mathbf{s}} \subset \mathcal{H} = \text{clos } \mathbb{T}_{\mathbf{r}} \text{ is (weakly) closed!}$$

Multi-linear ansatz destroys convexity, but existence of minimizers follows from Hackbusch & Falco

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Compare: Existence of Hartree Fock (Lieb & Simon, J.L. Lions) and of MCSCF (Friesecke, Levin) But: even the best rank 1 approximation of U is NP hard to compute! (Lim (2011))

Optimization by relaxation in TT format ALS

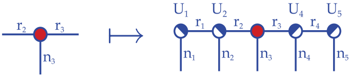
Alternating Linear Scheme - ALS

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

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

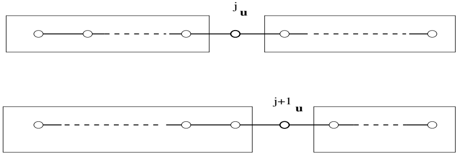
1. fix all component tensors $\mathbf{U}_\nu$, $\nu \in \{1, \ldots, d\} \setminus \{j\}$, except index j.

$\mathbf{P}_{i,1,U}$:



2. Optimize $\mathbf{U}_j(k_{j-1}, x_j, k_j)$, and orthogonalize left

Repeat the relaxation procedure (in the opposite direction.)



Relaxation scheme $\mathbf{U}(x_\nu)_{k_{\nu-1}}^{k_\nu}$

This is NOT exactly the DMRG algorithm!

A modified relaxation algorithm MALS

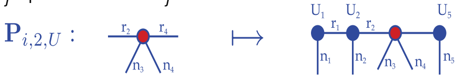
Disadvantage of simple relaxation:

1. $\mathbf{U}_j, \ldots$ must be (left)-orthogonalized,
2. $\mathbf{r} = (r_1, \ldots r_d)$ is fixed, but we want an adaptive rank selection

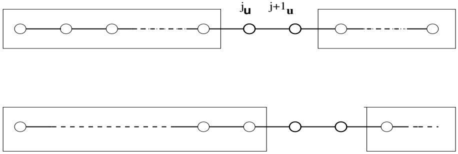
Modified Alternating Linear Scheme MALS (DMRG)

Idea: optimize comprised components

$U_{i,i+1} =: \left[\mathbf{W}(k_{j-1}, x_j, x_{j+1}, k_{j+1})\right] \approx \sum_{k_j=1}^{r_j} \left[\mathbf{U}(x_j)\right]_{k_{j-1}}^{k_j} \left[\mathbf{V}(x_{j+1})\right]_{k_j}^{k_{j+1}} \in \mathbb{R}^{r_{i-1} n_i n_{i+1} r_{i+1}}$.



system ⊗ 2 sites ⊗ environment



repeat in opposite direction ⇐

Retractions, extensions and density matrices

Let $x_i \mapsto \mathbf{W}_i(x_i) \in \mathbb{R}^{r_{i-1} \cdot n_i \cdot r_i}$ be of the size of a component tensor. The extension or dressing operator

$$\mathbf{P}_{i,1,U} := \mathbf{E}_i := \mathbf{E}_i(U) : X \to \mathbb{T}_{\mathbf{r}} \subset \mathcal{H} \ ,$$

extending W_i to a TT tensor in $\mathcal{H} = \bigotimes_{i=1}^{d} \mathbb{R}^{n_i}$, is defined by

$$\mathbf{W}_i(x_i) \mapsto \mathbf{E}_i \mathbf{W}_i(\mathbf{x}) := \mathbf{U}_1(x_1) \cdots \mathbf{W}_i(x_i) \cdots \mathbf{U}_d(x_d) \ .$$

The adjoint operator is $\mathbf{E}_i^T$. $\mathbf{P}_{i,2,U} := \mathbf{E}_{i,i+1}$ is defined analogously.
The left inverse $\mathbf{E}_i^{\dagger}$ applied to the tensor $U = \mathbf{U}_1 \cdots \mathbf{U}_i \cdots \mathbf{U}_d \in \mathbb{T}_{\mathbf{r}}$ is given by

$$\mathbf{U}_i = \mathbf{E}_i^{\dagger} U = (\mathbf{E}_i^T \mathbf{E}_i)^{-1} \mathbf{E}_i^T U \ .$$

E.g, if $\mathbf{U}_i$, $i = 1, \ldots, d-1$, are left orthogonal, the i−th density matrix will be defined by

$$\mathbf{I} \otimes \mathbf{D}_i := (\mathbf{E}_i^T \mathbf{E}_i)^{-1} \ .$$

Relaxation TT- ALS algorithm

Require: Functional $F : \mathbb{R}^{n_1 \times \ldots \times n_d} \to \mathbb{R}$, component starting vector $(U_1, \ldots, U_d)$.

Right-orthogonalise the components $(U_2, \ldots, U_d)$.

while termination criterion is not fulfiled **do**

  for $i = 1, \ldots, d-1$ **do**

    Find $\hat{U}_i = \text{argmin } F \circ \mathbf{E}_i \ : \ \mathbb{R}^{r_{i-1} \times n_i \times r_i} \to \mathbb{R}$.

    Set $U_i, U_{i+1} \leftarrow \hat{U}_i, U_{i+1}$, by applying an orthogonalisation.

  end for

  for $i = d, \ldots, 2$ **do**

    Find $\hat{U}_i = \text{argmin } F \circ \mathbf{E}_i : \ \mathbb{R}^{r_{i-1} \times n_i \times r_i} \to \mathbb{R}$.

    Set $U_i, U_{i-1} \leftarrow \hat{U}_i, U_{i-1}$, by applying an orthogonalisation.

  end for

end while

Modified relaxation TT- MALS algorithm (DMRG).

Require: Functional : $\mathbb{R}^{n_1 \times \dots \times n_d} \to \mathbb{R}$, component starting vector $(U_1, \dots, U_d)$.

Right-orthogonalise the components $(U_2, \dots, U_d)$.

while termination criterion is not fulfilled **do**

  for $i = 1, \dots, d-1$ **do**

    (Optimization step) Find

$(k_{i-1}, x_i, x_{i+1}, k_{i+1}) \mapsto W_i(k_{i-1}, x_i, x_{i+1}, k_{i+1})$ where

$$W_i = \text{argmin } F \circ \mathbf{W}_{i,i+1} \ : \ \mathbb{R}^{r_{i-1} \times n_i n_{i+1} \times r_{i+1}} \to \mathbb{R}.$$

    (Decimation step) Approximate with low rank r_i

$$\mathbf{W}_{k_{i-1},x_i}^{x_{i+1},k_{i+1}} \approx \sum_{k_i} \mathbf{U}_{k_{i-1},x_i}^{k_i} \mathbf{V}_{k_i}^{x_{i+1},k_{i+1}} \ .$$

  end for

  Repeat with reverse order

end while

ALS - Stationary conditions (equations)

For fixed j, and $Ax = B$ the stationary condition is

$$\boxed{\widetilde{\mathbf{A}}_{\mathbf{j}} \, \mathbf{U}_j = \mathbf{E}_j^T A \mathbf{E}_j \, \mathbf{U}_j = \mathbf{b}_j = \mathbf{E}_j B \ .}$$

For the eigenvalue problem

$$\boxed{\widetilde{\mathbf{A}}_{\mathbf{j}} \, \mathbf{U}_j = \mathbf{E}_j^T A \mathbf{E}_j \, \mathbf{U}_j = \lambda \widetilde{\mathbf{M}}_j \mathbf{U}_j = \lambda \mathbf{E}_j^T \mathbf{E}_j \, \mathbf{U}_j \ .}$$

For MALS we obtain

$$\widetilde{\mathbf{A}}_{\mathbf{j}} = \mathbf{E}_{j,j+1}^T A \mathbf{E}_{j,j+1} \quad , \quad \widetilde{\mathbf{M}}_{\mathbf{j}} = \mathbf{E}_{j,j+1}^T \mathbf{E}_{j,j+1}$$

Lemma (Rohw. & Holtz & S.)

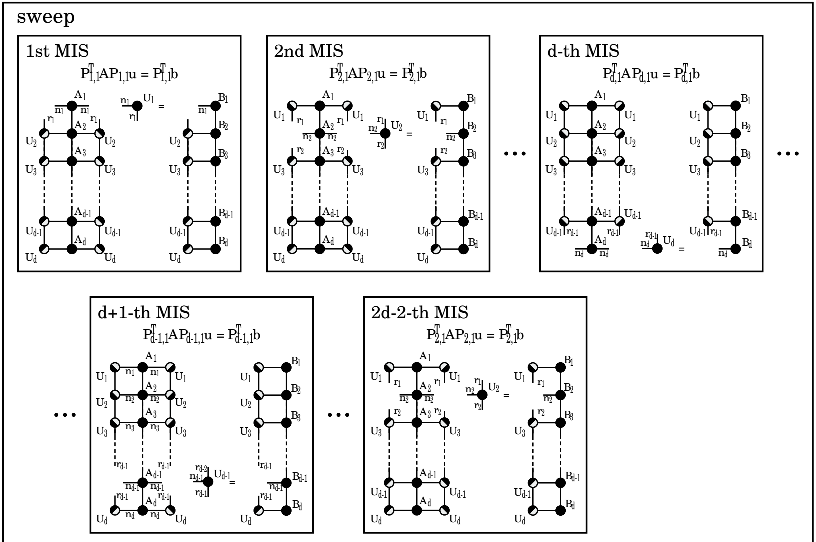
If $\mathbf{U}_j$, $j < i$ *are left-, and* $\mathbf{U}_j$, $i < j$ *are right-orthogonal then*

$$\mathit{cond}\, \widetilde{\mathbf{A}}_{\mathbf{i}} \leq \ \mathit{cond}\, A \ \ \mathit{and} \ \ \widetilde{\mathbf{M}}_{\mathbf{i}} = \mathbf{I} \ !$$

Remark: $\det \mathbf{A}_i \neq 0$ can hold, for some A when $\det A = 0$
(-RIP, compressed sensing)

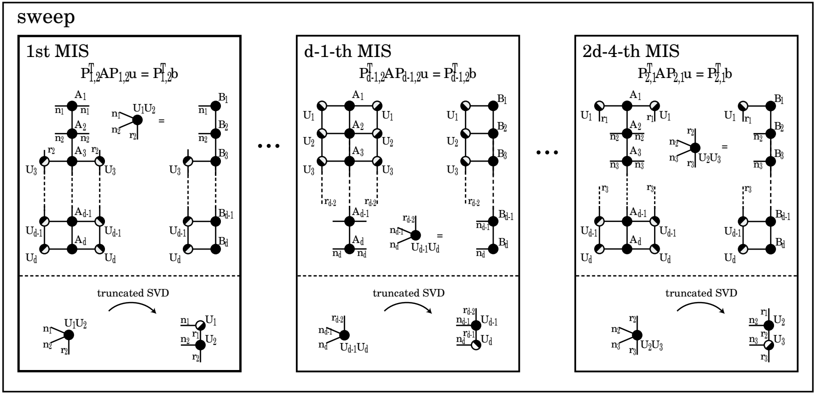
ALS - Solution scheme for linear equations $Ax = b$

- Proceeding in “sweeps”: Solution of successive linear systems
- additional orthogonalisation



MALS - Solution scheme for linear equations $Ax = b$ (inspired by the DMRG algorithm)

- Proceeding in "sweeps": Solution of successive linear systems for comprised components $U_{i,i+1} \in \mathbb{R}^{r_{i-1} n_i n_{i+1} r_{i+1}}$, other components fixed
- subsequent SVDs restore orthogonal TT-format



ALS - Stationary conditions

$$\mathbf{G}_j := \left[\mathbf{g}_{k_{j-1}}^{k'_{j-1}}\right] = \langle \mathbf{L}^{k_{j-1}}, \mathbf{A}_L \mathbf{L}^{k'_{j-1}} \rangle \ ,$$

$$\mathbf{H}_j := \left[\mathbf{h}_{k_j}^{k'_j}\right] = \langle \mathbf{R}_{k_j}, \mathbf{A}_R \mathbf{R}_{k'_j} \rangle \ ,$$

$$\mathbf{X}_j = \left[\mathbf{p}_{k_{j-1}}^{k'_{j-1}}\right] = \langle \mathbf{L}^{k_{j-1}}, \mathbf{L}^{k'_{j-1}} \rangle \ , \ \mathbf{Q}_j := \left[\mathbf{q}_{k_j}^{k'_j}\right] = \langle \mathbf{R}_{k_j}, \mathbf{R}_{k'_j} \rangle \ .$$

$$\langle \mathbf{e}_i, \mathbf{b}_{k_{j-1}}^{k_j} \rangle := \langle B, \mathbf{L}^{k_{j-1}} \otimes \mathbf{e}_i \otimes \mathbf{R}_{k_j} \rangle \ ,$$

and let $\mathbf{u}_j := \left[u_{k_{j-1},x_j,k_j}\right]$, $\mathbf{b} := \left[b_{k_{j-1},x_j,k_j}\right]$
For fixed j, and $Ax = B$ the stationary condition is

$$\boxed{\widetilde{\mathbf{A}}_{\mathbf{j}} \, \mathbf{u}_j = (\mathbf{G}_j \otimes \mathbf{a}_j \otimes \mathbf{H}_j) \, \mathbf{u}_j = \mathbf{b}_j \ .} \quad *$$

and for the eigenvalue problem

$$\boxed{\widetilde{\mathbf{A}}_j \mathbf{u}_j := (\mathbf{G}_j \otimes \mathbf{a}_j \otimes \mathbf{H}_j) \mathbf{u}_j = \lambda \widetilde{\mathbf{M}}_j \mathbf{u}_j = \lambda (\mathbf{X}_j \otimes \mathbf{I} \otimes \mathbf{Q}_j) \mathbf{u}_j \ .} \quad *$$

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

Stationary condition

Defining the matrices

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

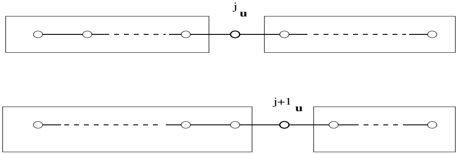
$$\mathbf{H} := \left((\mathbf{h})_{k_j}^{k'_j}\right) = \langle \mathbf{r}_{k_j}, \mathbf{A}_R \mathbf{r}_{k'_j} \rangle \ ,$$

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

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

* Rank $\mathbf{A} = 1$

Update $j \to j+1$



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

$$g^{k'_j}_{k_j} = \sum_{x_j, y_j = 1}^{n} \sum_{k_{j-1}, k'_{j-1} = 0}^{r_{j-1}} u^{k_j}_{x_j, k_{j-1}} g^{k'_{j-1}}_{k_{j-1}} a^{y_j}_{x_j} u^{k'_j}_{y_j, k'_{j-1}} \ . \qquad *$$

shortly

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

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

* Rank $\mathbf{A} = 1$

Theorem (reconstruction)

Let the initial guess $U^{(0)} \in \mathbb{T}^{\mathbf{r}}$ does not provide rank deficiencies, e.g. be sufficiently close to

$$U = \text{ argmin} \left\{ F(V) := \frac{1}{2} \langle V - b, V - b \rangle : V \in \mathbb{T}^{\mathbf{r}} \right\} .$$

And if $U = b$, with $U \in \mathbb{T}^{\mathbf{r}}$ (reconstruction), then the ALS scheme $U^{(n)} \in \mathbb{T}^{\mathbf{r}}$ terminates after the first half sweep.

Theorem (approximation)

Let the initial guess $U^{(0)} \in \mathbb{T}^{\mathbf{r}}$ be sufficiently close to

$$U = \text{ argmin} \left\{ F(V) := \frac{1}{2} \langle AV - 2f, V \rangle : V \in \mathbb{T}^{\mathbf{r}} \right\} .$$

Let $A : \mathcal{H} \to \mathcal{H}$ be SPD, and $W \in \mathcal{H}$ solving $AW = f$, and $\|W - U\| \leq \delta$ sufficiently small. Then the ALS converges linearly

$$\|U - U^{(n+1)}\| \leq L \|U - U^{(n)}\| \, , \; 0 < L < 1 \, .$$

Scetch of proof

Suppose $U \in N_\delta(0)$ and let $N_\delta(0)$ be a suitable neighbourhood of $U^{(n)}$. Let $\mathbf{u} := (\mathbf{w}_1, \ldots, \mathbf{w}_d) \in X := X_{\underline{r}}$ and assume a (local) parametrization $U = T(\mathbf{u})$ (details later).

We assume $A : \mathcal{H} \to \mathcal{H}$ is SPD and consider

$$J(\mathbf{u}) := F(T(\mathbf{u})) = \frac{1}{2}\langle AT(\mathbf{u}), T(\mathbf{u})\rangle - \langle f, T(\mathbf{u})\rangle \ .$$

First order condition reads as

$$\big[J'(\mathbf{u})\big](v) = \Big\langle AT(\mathbf{u}) - f, \ \ \big[T'(\mathbf{u})\big](\mathbf{v})\Big\rangle = 0 \ \ \forall \mathbf{v} \in X,$$

For ALS, i.e. non-linear Gauß-Seidel, we have to show that the corresp.Hessian is SPD:

$$\begin{aligned}\big[J''(\mathbf{u})\big](\mathbf{v},\mathbf{v}) \ \ &= \ \ \Big\langle A\big[T'(\mathbf{u})\big](\mathbf{v}), \ \big[T'(\mathbf{u})\big](\mathbf{v})\Big\rangle \\ &\quad + \Big\langle AT(\mathbf{u}) - f, \big[T''(\mathbf{u})\big](\mathbf{v},\mathbf{v})\Big\rangle \geq \gamma \|\mathbf{v}\|^2 \ \ \forall \mathbf{v} \in X \ .\end{aligned}$$

If the residual $F'(T(\mathbf{u})) = AT(\mathbf{u}) - f = AU - f \in \mathcal{H}$ is sufficiently small, e.g $= 0$ (reconstruction), this remains to be true, due to the SPD operator A.

Complexity - rough estimates

MALS $\approx$ DMRG:

- storage components $\mathcal{O}(n^2 d r^2)$
- storage matrices $\mathcal{O}(n^2 d R_c r^2)$
- computation $\mathcal{O}(n^2 d R_c r^3)$

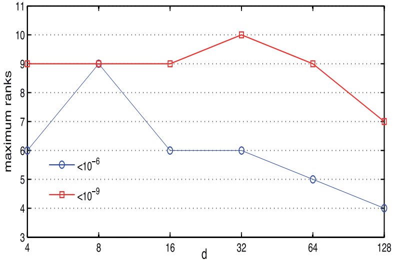
if R_c is a canonical rank of A.
If A is represented in TT with maximal TT rank R. then

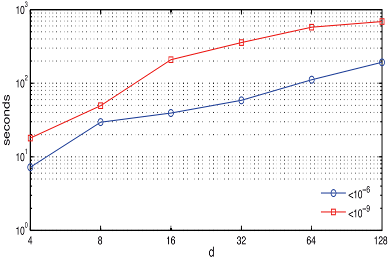
- storage components $\mathcal{O}(n^2 d r^2)$
- storage matrices $\mathcal{O}(n^2 d R^2 r^2)$
- computation $\mathcal{O}(n^2 d R^3 r^3)$

For ALS (one-site DMRG) n^2 is replaced by n.

Solution of $-\Delta U = b$

- Dimension $d = 4, \ldots, 128$ varying
- Gridsize $n = 10$
- Right-hand-side b of rank 1
- Solution U has rank 13





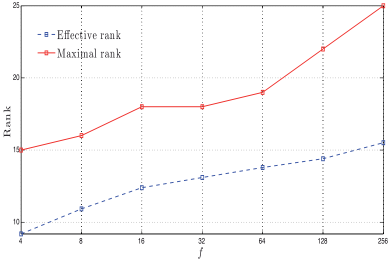
Example: Eigenvalue problem in QTT

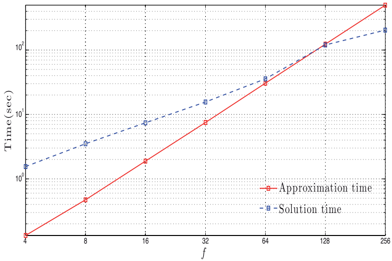
in courtesy of B. Khoromskij, I. Oseledets, *QTT: Toward bridging high-dimensional quantum molecular dynamics and DMRG methods*,

$$H\Psi = (-\frac{1}{2}\Delta + V)\Psi = E\Psi$$

with potential energy surface given by Henon-Heiles potential

$$V(q_1, \ldots, q_f) = \frac{1}{2}\sum_{k=1}^{f} q_k^2 + \lambda \sum_{k=1}^{f-1}\left(q_k^2 q_{k+1} - \frac{1}{3}q_k^3\right).$$





Dimensions $f = 4, \ldots, 256$; 1-D grid size $n = 128 = 2^7 = 2^d$; $\rightsquigarrow$

$$\text{QTT-tensors} \in \bigotimes_{i=1}^{7f} \mathbb{R}^2 = \mathbb{R}^{\overbrace{2 \times .. \times 2}^{7f=1792}}.$$

Thank you for your attention.

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