Low-Rank Tensor Methods for Symmetric Eigenvalue Problems

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Introduction

Solve a *symmetric eigenvalue problem*

$$\mathcal{A}u(x) = \lambda u(x), \quad x \in \Omega \subset \mathbb{R}^d.$$

in an appropriate function space over Ω.

Discretization on a $n_1 \times n_2 \times \cdots \times n_d$ tensor grid yields the matrix eigenvalue problem

$$A\underline{u} = \lambda \underline{u}, \qquad \underline{u} \in \mathbb{R}^N, \text{ with } N = n_1 n_2 \cdots n_d.$$

For d large **we cannot:**

- store and access the grid vector $\underline{u}$.
- perform matrix-vector multiplication $A\underline{u}$.

Introduction

- **Example:** Electronic Schrödinger equation $H\psi = E\psi$ for a system of N electrons and K atoms

$$H = \frac{1}{2}\sum_{i=1}^{N} \Delta_i - \sum_{i=1}^{N} \left(\sum_{I=1}^{K} \frac{Z_I}{\|x_i - x_I\|} + \sum_{j \neq i}^{N} \frac{1}{\|x_i - x_j\|} \right)$$

  operates on antisymmetric functions $\psi \in H^1(\mathbb{R}^{3N})$. Discretization on a tensor grid with n points along each coordinate:

$$\Rightarrow \quad \text{Compute eigenvalues of a matrix with size } n^{3N} \times n^{3N}$$

  So-called **curse of dimensionality**.

- Exploit the low-rank approximability of the solution.

Low-Rank Matrices

Example: The matrix case $d = 2$

- Consider the grid function $\mathbf{u}(i_1, i_2) = u(x_{i_1}, y_{i_2})$ as $n_1 \times n_2$ matrix
- Assume the eigenvector for the smallest eigenvalue has rank $r \ll \min(n_1, n_2)$:

$$\mathrm{vec}(\mathbf{u}) = \mathrm{vec}(UV^{\mathsf{T}}), \qquad U \in \mathbb{R}^{n_1 \times r}, V \in \mathbb{R}^{n_2 \times r}$$

	$\mathbf{u}$	UV^{T}
Storage required:	$n_1 n_2$	$(n_1 + n_2)r$

Low-Rank Matrices

Rewrite the *Rayleigh quotient* for the eigenvalue system in terms of U, V using the Kronecker product:

$$\frac{\mathrm{vec}(\mathbf{u})^\mathsf{T} A\,\mathrm{vec}(\mathbf{u})}{\mathrm{vec}(\mathbf{u})^\mathsf{T}\,\mathrm{vec}(\mathbf{u})} = \frac{\mathrm{vec}(UV^\mathsf{T})^\mathsf{T} A\,\mathrm{vec}(UV^\mathsf{T})}{\mathrm{vec}(UV^\mathsf{T})^\mathsf{T}\,\mathrm{vec}(UV^\mathsf{T})}$$

$$\text{reduced EVP for U} \longrightarrow = \frac{\mathrm{vec}(U)^\mathsf{T}(V \otimes I)^\mathsf{T} A (V \otimes I)\mathrm{vec}(U)}{\mathrm{vec}(U)^\mathsf{T}(V^\mathsf{T}V \otimes I)\mathrm{vec}(U)}$$

$$\text{reduced EVP for V} \longrightarrow = \frac{\mathrm{vec}(V^\mathsf{T})^\mathsf{T}(I \otimes U)^\mathsf{T} A (I \otimes U)\mathrm{vec}(V^\mathsf{T})}{\mathrm{vec}(V^\mathsf{T})^\mathsf{T}(I \otimes U^\mathsf{T}U)\mathrm{vec}(V^\mathsf{T})}$$

Alternate optimization between U and V^T to solve the original eigenvalue problem.

Low-Rank Tensors: TT/MPS format

Matrix Product States (MPS) [Fannes et al. 1992, Östlund/Rommer 1995]
Tensor Train (TT) [Oseledets/Tyrtyshnikov 2009, Oseledets 2011]

$$\mathbf{u}(i_1, i_2, \ldots, i_d) = U_1(i_1)U_2(i_2)\cdots U_d(i_d)$$

with the μth matrix $(\mu = 1, \ldots, d)$:

$$U_\mu(i_\mu) = \mathbb{R}^{r_{\mu-1}\times r_\mu}, \quad r_0 = r_d = 1.$$

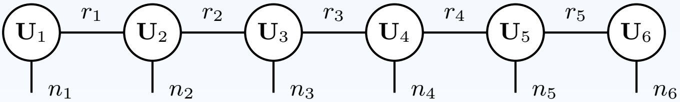
or equivalently in terms of the *core tensors* $\mathbf{U}_\mu \in \mathbb{R}^{r_{\mu-1}\times n_\mu \times r_\mu}$:

$$\mathbf{u}(i_1, \ldots, i_d) = \sum_{j_1=1}^{r_1} \cdots \sum_{j_{d-1}=1}^{r_{d-1}} \mathbf{U}_1(1, i_1, j_1)\mathbf{U}_2(j_1, i_2, j_2)\cdots \mathbf{U}_d(j_{d-1}, i_d, 1).$$

The $U_\mu(i_\mu)$ are slices of the **core tensors**:

$$U_\mu(i_\mu) = \mathbf{U}_\mu(:, i_\mu, :)$$

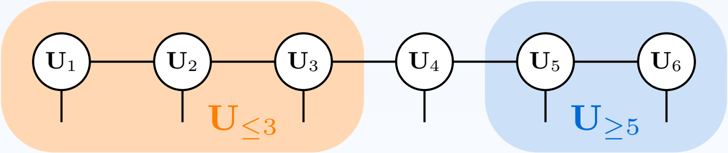
Low-Rank Tensors: TT/MPS format



The minimum ranks r_μ needed for an exact representation are

$$r_\mu = \operatorname{rank}\left(\operatorname{reshape}\left(\mathbf{u}, \mathbb{R}^{(n_1\cdots n_{\mu-1})\times(n_\mu\cdots n_d)}\right)\right)$$

Low-Rank Tensors: TT/MPS format



The minimum ranks r_μ needed for an exact representation are

$$r_\mu = \operatorname{rank}\left(\operatorname{reshape}\left(\mathbf{u}, \mathbb{R}^{(n_1 \cdots n_{\mu-1}) \times (n_\mu \cdots n_d)}\right)\right)$$

For every core $\mathbf{U}_\mu$ we have:

- $\mathbf{u} \in \operatorname{ran}(\mathbf{U}_{\leq \mu-1}) \otimes \mathbb{R}^{n_\mu} \otimes \operatorname{ran}(\mathbf{U}_{\geq \mu+1})$
- $\operatorname{vec}(\mathbf{u}) = \mathcal{U}_{\neq \mu} \operatorname{vec}(\mathbf{U}_\mu), \quad \mathcal{U}_{\neq \mu} = \mathbf{U}_{\leq \mu-1} \otimes I_{n_\mu} \otimes \mathbf{U}_{\geq \mu+1}$

Operator TT format

Low-rank structure of $\mathbf{u}$ is useless unless we can use it in the multiplication with operator A

Operator TT format [Oseledets 2011]

$$A(i_1, \ldots i_d, j_1, \ldots j_d) = A_1(i_1, j_1) A_2(i_2, j_2) \cdots A_d(i_d, j_d),$$

$$\text{with} \quad A_\mu(i_\mu, j_\mu) \in \mathbb{R}^{s_{\mu-1} \times s_\mu}$$

Application to TT tensor:

$$\mathbf{v} = A\mathbf{u} \quad \Leftrightarrow \quad \text{“ } \mathbf{V}_\mu = \mathbf{A}_\mu \mathbf{U}_\mu \text{ ” } \textit{(suitably reshaped)}$$

Ranks multiply!

Operator TT format

Example: d-dimensional discrete Laplacian,

$$L = \sum_{i=1}^{d} I_d \otimes \cdots \otimes L_\mu \otimes \cdots \otimes I_1,$$

with L_μ the one-dim. finite difference matrix, can be represented as TT operator of rank 2: [Kazeev/Khoromskij 2012]

$$A_1(i_1, j_1) = \begin{bmatrix} L_1(i_1, j_1) & I_1(i_1, j_1) \end{bmatrix}, \quad A_d(i_d, j_d) = \begin{bmatrix} I_d(i_d, j_d) \\ L_d(i_d, j_d) \end{bmatrix},$$

and

$$A_\mu(i_\mu, j_\mu) = \begin{bmatrix} I_\mu(i_\mu, j_\mu) & 0 \\ L_\mu(i_\mu, j_\mu) & I_\mu(i_\mu, j_\mu) \end{bmatrix}, \quad \mu = 2, \ldots, d-1.$$

ALS algorithm for smallest EV

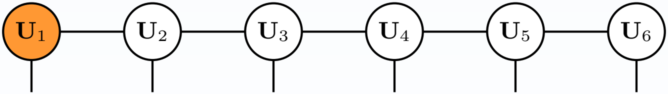
Just like in the matrix case:

$$\frac{\mathrm{vec}(\mathbf{u})^\mathsf{T} A\,\mathrm{vec}(\mathbf{u})}{\mathrm{vec}(\mathbf{u})^\mathsf{T}\,\mathrm{vec}(\mathbf{u})} = \frac{\mathrm{vec}(\mathbf{U}_\mu)^\mathsf{T}\mathcal{U}_{\neq\mu}^\mathsf{T} A\,\mathcal{U}_{\neq\mu}\mathrm{vec}(\mathbf{U}_\mu)}{\mathrm{vec}(\mathbf{U}_\mu)^\mathsf{T}\mathcal{U}_{\neq\mu}^\mathsf{T}\mathcal{U}_{\neq\mu}\mathrm{vec}(\mathbf{U}_\mu)}$$

Note: We can choose $\mathcal{U}_{\neq\mu}$ orthogonal.

Algorithm: Cycle through each core $\mathbf{U}_\mu$ and solve for each the reduced EVP with matrix

$$A_1 = \mathcal{U}_{\neq 1}^\mathsf{T} A\,\mathcal{U}_{\neq 1} \;\in \mathbb{R}^{(r_0 n_1 r_1)\times(r_0 n_1 r_1)}.$$



The ranks r_μ do not change! Need a-priori knowledge?

ALS algorithm for smallest EV

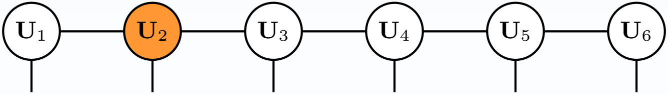
Just like in the matrix case:

$$\frac{\mathrm{vec}(\mathbf{u})^\mathsf{T} A\,\mathrm{vec}(\mathbf{u})}{\mathrm{vec}(\mathbf{u})^\mathsf{T}\,\mathrm{vec}(\mathbf{u})} = \frac{\mathrm{vec}(\mathbf{U}_\mu)^\mathsf{T}\mathcal{U}_{\neq\mu}^\mathsf{T} A\,\mathcal{U}_{\neq\mu}\mathrm{vec}(\mathbf{U}_\mu)}{\mathrm{vec}(\mathbf{U}_\mu)^\mathsf{T}\mathcal{U}_{\neq\mu}^\mathsf{T}\mathcal{U}_{\neq\mu}\mathrm{vec}(\mathbf{U}_\mu)}$$

Note: We can choose $\mathcal{U}_{\neq\mu}$ orthogonal.

Algorithm: Cycle through each core $\mathbf{U}_\mu$ and solve for each the reduced EVP with matrix

$$A_2 = \mathcal{U}_{\neq 2}^\mathsf{T} A\,\mathcal{U}_{\neq 2} \;\in \mathbb{R}^{(r_1 n_2 r_2)\times(r_1 n_2 r_2)}.$$



The ranks r_μ do not change! Need a-priori knowledge?

ALS algorithm for smallest EV

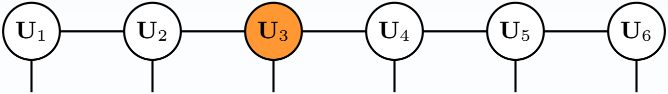
Just like in the matrix case:

$$\frac{\mathrm{vec}(\mathbf{u})^\mathsf{T} A\,\mathrm{vec}(\mathbf{u})}{\mathrm{vec}(\mathbf{u})^\mathsf{T}\,\mathrm{vec}(\mathbf{u})} = \frac{\mathrm{vec}(\mathbf{U}_\mu)^\mathsf{T}\mathcal{U}_{\neq\mu}^\mathsf{T} A\,\mathcal{U}_{\neq\mu}\mathrm{vec}(\mathbf{U}_\mu)}{\mathrm{vec}(\mathbf{U}_\mu)^\mathsf{T}\mathcal{U}_{\neq\mu}^\mathsf{T}\mathcal{U}_{\neq\mu}\mathrm{vec}(\mathbf{U}_\mu)}$$

Note: We can choose $\mathcal{U}_{\neq\mu}$ orthogonal.

Algorithm: Cycle through each core $\mathbf{U}_\mu$ and solve for each the reduced EVP with matrix

$$A_3 = \mathcal{U}_{\neq 3}^\mathsf{T} A\,\mathcal{U}_{\neq 3} \ \in \mathbb{R}^{(r_2 n_3 r_3)\times(r_2 n_3 r_3)}.$$



The ranks r_μ do not change! Need a-priori knowledge?

ALS algorithm for smallest EV

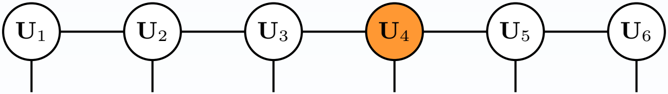
Just like in the matrix case:

$$\frac{\mathrm{vec}(\mathbf{u})^\mathsf{T} A\, \mathrm{vec}(\mathbf{u})}{\mathrm{vec}(\mathbf{u})^\mathsf{T}\, \mathrm{vec}(\mathbf{u})} = \frac{\mathrm{vec}(\mathbf{U}_\mu)^\mathsf{T} \mathcal{U}_{\neq\mu}^\mathsf{T} A\, \mathcal{U}_{\neq\mu} \mathrm{vec}(\mathbf{U}_\mu)}{\mathrm{vec}(\mathbf{U}_\mu)^\mathsf{T} \mathcal{U}_{\neq\mu}^\mathsf{T} \mathcal{U}_{\neq\mu} \mathrm{vec}(\mathbf{U}_\mu)}$$

Note: We can choose $\mathcal{U}_{\neq\mu}$ orthogonal.

Algorithm: Cycle through each core $\mathbf{U}_\mu$ and solve for each the reduced EVP with matrix

$$A_4 = \mathcal{U}_{\neq 4}^\mathsf{T} A\, \mathcal{U}_{\neq 4} \; \in \mathbb{R}^{(r_3 n_4 r_4)\times(r_3 n_4 r_4)}.$$



The ranks r_μ do not change! Need a-priori knowledge?

ALS algorithm for smallest EV

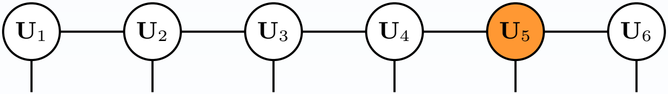
Just like in the matrix case:

$$\frac{\mathrm{vec}(\mathbf{u})^\mathsf{T} A \,\mathrm{vec}(\mathbf{u})}{\mathrm{vec}(\mathbf{u})^\mathsf{T}\,\mathrm{vec}(\mathbf{u})} = \frac{\mathrm{vec}(\mathbf{U}_\mu)^\mathsf{T} \mathcal{U}_{\neq\mu}^\mathsf{T} A \,\mathcal{U}_{\neq\mu} \mathrm{vec}(\mathbf{U}_\mu)}{\mathrm{vec}(\mathbf{U}_\mu)^\mathsf{T} \mathcal{U}_{\neq\mu}^\mathsf{T} \mathcal{U}_{\neq\mu} \mathrm{vec}(\mathbf{U}_\mu)}$$

Note: We can choose $\mathcal{U}_{\neq\mu}$ orthogonal.

Algorithm: Cycle through each core $\mathbf{U}_\mu$ and solve for each the reduced EVP with matrix

$$A_5 = \mathcal{U}_{\neq 5}^\mathsf{T} A \,\mathcal{U}_{\neq 5} \;\in \mathbb{R}^{(r_4 n_5 r_5)\times(r_4 n_5 r_5)}.$$



The ranks r_μ do not change! Need a-priori knowledge?

ALS algorithm for smallest EV

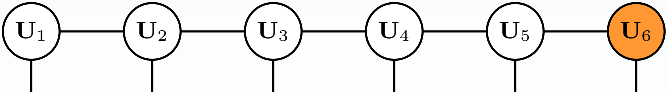
Just like in the matrix case:

$$\frac{\mathrm{vec}(\mathbf{u})^\mathsf{T} A\,\mathrm{vec}(\mathbf{u})}{\mathrm{vec}(\mathbf{u})^\mathsf{T}\,\mathrm{vec}(\mathbf{u})} = \frac{\mathrm{vec}(\mathbf{U}_\mu)^\mathsf{T}\mathcal{U}_{\neq\mu}^\mathsf{T} A\,\mathcal{U}_{\neq\mu}\mathrm{vec}(\mathbf{U}_\mu)}{\mathrm{vec}(\mathbf{U}_\mu)^\mathsf{T}\mathcal{U}_{\neq\mu}^\mathsf{T}\mathcal{U}_{\neq\mu}\mathrm{vec}(\mathbf{U}_\mu)}$$

Note: We can choose $\mathcal{U}_{\neq\mu}$ orthogonal.

Algorithm: Cycle through each core $\mathbf{U}_\mu$ and solve for each the reduced EVP with matrix

$$A_6 = \mathcal{U}_{\neq 6}^\mathsf{T} A\,\mathcal{U}_{\neq 6} \;\in \mathbb{R}^{(r_5 n_6 r_6)\times(r_5 n_6 r_6)}.$$



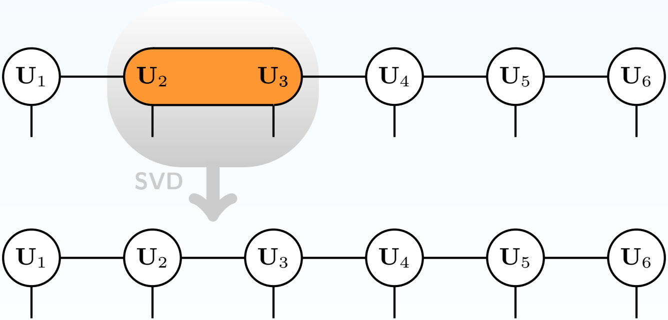
The ranks r_μ do not change! Need a-priori knowledge?

DMRG algorithm for smallest EV

Make the algorithm **rank adaptive** by optimizing neighboring cores together: **(DMRG)** [White 1992]

Solve for each the reduced EVP with matrix

$$A_{\mu,\mu+1} = \mathcal{U}_{\neq\mu,\mu+1}^{\mathsf{T}} A \mathcal{U}_{\neq\mu,\mu+1} \in \mathbb{R}^{(r_{\mu-1}n_\mu n_{\mu+1}r_{\mu+1})\times(r_{\mu-1}n_\mu n_{\mu+1}r_{\mu+1})}.$$



Good, but can easily become prohibitively expensive.

Computing several eigenvectors

Compute p smallest eigenvalues and eigenvectors by **trace minimization:**

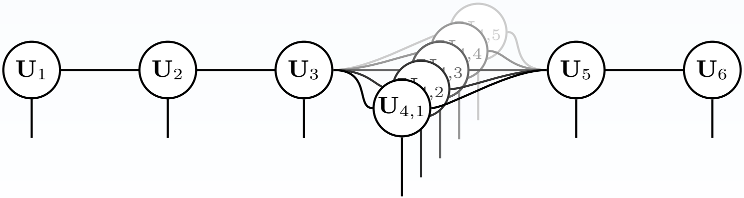
$$\min \operatorname{trace}(\mathbf{U}^T A \mathbf{U}), \quad \mathbf{U}^\mathsf{T}\mathbf{U} = I_p,$$

$$\mathbf{U} = [\operatorname{vec}(\mathbf{u}_1), \operatorname{vec}(\mathbf{u}_2), \ldots, \operatorname{vec}(\mathbf{u}_p)]$$

Use seperate TT-representation for each $\mathbf{u}_\alpha, \alpha = 1, \ldots, p$? Better:

Block-μ TT format [Pižorn/Verstraete 2012, Dolgov et al. 2013]

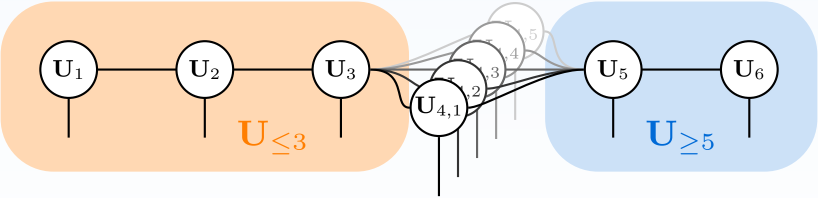
$$\mathbf{u}_\alpha(i_1, i_2, \ldots, i_d) = U_1(i_1) \cdots U_{\mu-1}(i_{\mu-1}) U_{\mu,\alpha}(i_\mu) U_{\mu+1}(i_{\mu+1}) \cdots U_d(i_d)$$



Block-TT format

For $\mathbf{U}$ in **block-μ TT format**, it holds:

- $\mathbf{u}_\alpha \in \operatorname{ran}(\mathbf{U}_{\leq \mu-1}) \otimes \mathbb{R}^{n_\mu} \otimes \operatorname{ran}(\mathbf{U}_{\geq \mu+1})$ independent of $\alpha = 1, \ldots, p$!
- $\mathbf{U} = \mathcal{U}_{\neq\mu} \mathbf{V}_\mu, \quad \mathbf{V}_\mu = [\operatorname{vec}(\mathbf{U}_{\mu,1}), \operatorname{vec}(\mathbf{U}_{\mu,2}), \ldots, \operatorname{vec}(\mathbf{U}_{\mu,p})]$

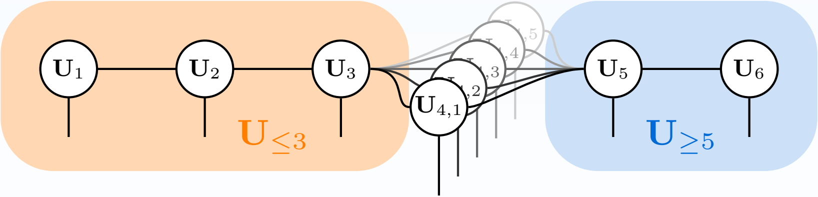


Block-TT format

Reduced problem for the p smallest eigenvalues:

If $\mathbf{U}$ is in block-μ format, and $\mathcal{U}_{\neq\mu}$ is orthogonal:

$$\min \operatorname{trace}(\mathbf{V}_\mu^\mathsf{T} \mathcal{U}_{\neq\mu}^\mathsf{T} A \mathcal{U}_{\neq\mu} \mathbf{V}_\mu), \quad \mathbf{V}_\mu \in \mathbb{R}^{r_{\mu-1} n_\mu r_\mu \times p}, \quad \mathbf{V}_\mu^\mathsf{T} \mathbf{V}_\mu = I_p,$$



Going from block-μ to block-$\mu + 1$

The position of multicore V_μ is *arbitrary* and can be *changed*:

1. Reshape $\mathbf{V}_\mu$ into matrix $\widetilde{\mathbf{V}}_\mu \in \mathbb{R}^{(r_{\mu-1}n_\mu)\times(pr_\mu)}$
2. Minimal-rank decomposition

$$\widetilde{\mathbf{V}}_\mu = Q \begin{bmatrix} P_1 & P_2 & \dots & P_p \end{bmatrix}, \quad Q \in \mathbb{R}^{r_{\mu-1}n_\mu \times s}, \quad P_\alpha \in \mathbb{R}^{s \times r_\mu}$$

3. Update cores

$$\mathbf{U}_\mu \leftarrow Q, \qquad \mathbf{U}_{\mu+1,\alpha} \leftarrow P_\alpha \mathbf{U}_{\mu+1},\ \alpha = 1, \dots, p$$

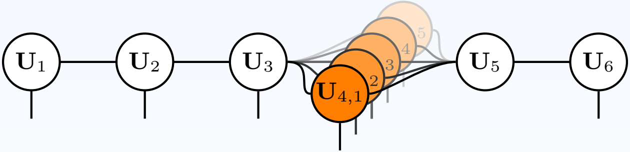
By this shifting procedure, the rank between the two cores has changed

$$r_\mu \leftarrow s$$

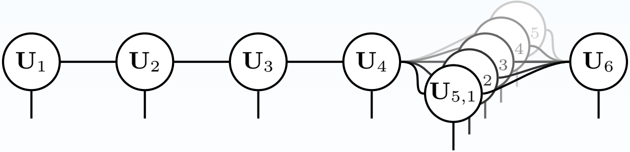
$\Rightarrow$ **Rank adaptivity** if $p > 1$: $\quad 0 < s \leq \min(r_{\mu-1}n_\mu, r_\mu p)$

Block-TT ALS algorithm for p eigenvalues

Optimize



Shift multicore to $\mu + 1$



[Dolgov et al. 2013]

Improving convergence: Subspace correction

Adding gradient information:

$$\mathbf{R} = A\mathbf{U} - \mathbf{U}\Lambda \quad \text{(the global residual)}$$

Add to the current intermediate result to enrich the subspace

$$\tilde{\mathbf{U}} = \mathbf{U} - \mathbf{R}$$

This also increases the rank in all modes:

$$\mathrm{rank}(\tilde{\mathbf{U}}) = \mathrm{rank}(\mathbf{U}) + \mathrm{rank}(\mathbf{R})$$

Too costly to enrich all cores with global gradient information after each step...

AMEn: Local subspace correction

Alternating Minimal Energy (AMEn) method for linear systems
[Dolgov/Savostyanov 2013]

- Start iteration with random TT tensor of rank one
- Add gradients for both acceleration and rank adaptivity of the algorithm
- But: Only inject the gradient information *locally* to cores $\mathbf{U}_\mu$ and $\mathbf{U}_{\mu+1}$.

Use the *projected DMRG (two-core) residual*

$$\mathbf{R}_{\mu,\mu+1} = \mathcal{U}_{\neq\mu,\mu+1}^{\mathsf{T}}(A\mathbf{U} - \mathbf{U}\Lambda)$$

Interpretation: Steepest Descent for DMRG

$$\mathcal{U}_{\neq\mu,\mu+1}^{\mathsf{T}}\tilde{\mathbf{U}} = \mathcal{U}_{\neq\mu,\mu+1}^{\mathsf{T}}\mathbf{U} - \mathbf{R}_{\mu,\mu+1}$$

Local subspace correction

How to augment with the projected DMRG (two-core) residual?

$$\mathbf{R}_{\mu,\mu+1} = \mathcal{U}_{\neq\mu,\mu+1}^{\mathsf{T}}(A\mathbf{U} - \mathbf{U}\Lambda)$$

(We can compute this efficiently)

First decompose into two parts:

$$R_{\mu,\mu+1,\alpha}(i_\mu, i_{\mu+1}) = R_{\mu,\alpha}(i_\mu)R_{\mu+1}(i_{\mu+1})$$

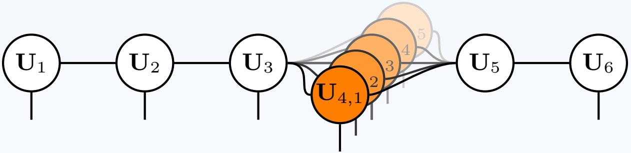
Then augment cores $\mathbf{U}_\mu$ and $\mathbf{U}_{\mu+1}$:

$$\tilde{U}_{\mu,\alpha}(i_\mu) = \begin{bmatrix} U_{\mu,\alpha}(i_\mu) & \\ & R_{\mu,\alpha}(i_\mu) \end{bmatrix}$$

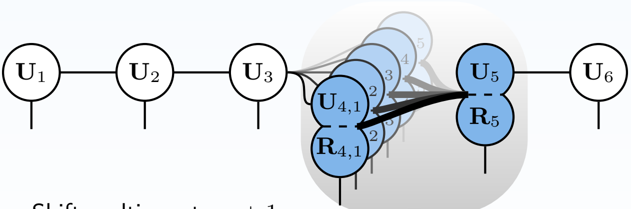
$$\tilde{U}_{\mu+1}(i_{\mu+1}) = \begin{bmatrix} U_{\mu+1}(i_{\mu+1}) & \\ & R_{\mu+1}(i_{\mu+1}) \end{bmatrix}$$

Our algorithm: Block ALS with local enrichment

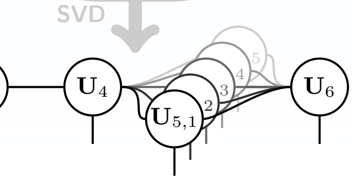
Optimize



Augment with (preconditioned) projected residual



Shift multicore to $\mu + 1$



Preconditioning the residual correction

Inject a preconditioner into the residual correction (think PINVIT)

$$\mathbf{R}_{\mu,\mu+1} = \mathcal{B}_{\mu,\mu+1}^{-1} \mathcal{U}_{\neq\mu,\mu+1}^{\mathsf{T}} (A\mathbf{U} - \mathbf{U}\Lambda)$$

where $\mathcal{B}_{\mu,\mu+1}^{-1}$ is a preconditioner for the local reduced problem.

Deriving a good preconditioner for the local problem can be challenging!

Numerical experiments

Model problem:

$$\begin{aligned} -\Delta u(x) + V(x)u(x) &= \lambda u(x), && \text{for } x \in \Omega = (a,b)^d \\ u(x) &= 0 && \text{for } x \in \delta\Omega \end{aligned}$$

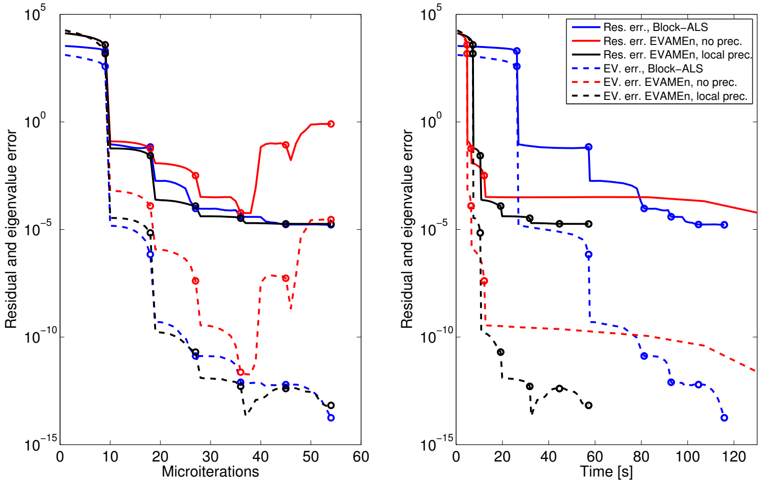
Newton potential:

$$V(x) = \frac{1}{\|x\|}$$

Approximated in low-rank TT format (rank 10) using exponential sums [Hackbusch 2010]

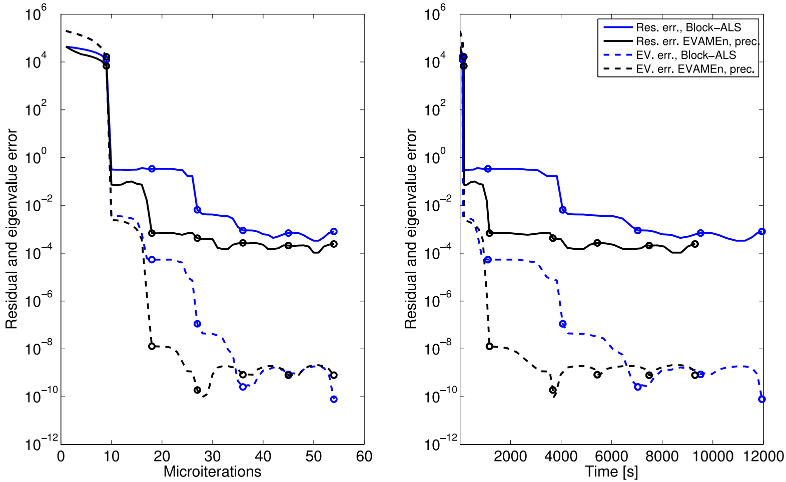
Preconditioner: Approximation of inverse of projected Laplacian by exponential sums (rank 3). [Grasedyk 2004, Hackbusch 2010]

Newton potential: One eigenvalue



$\Omega = (-1, 1)^{10}, n = 128 \rightarrow$ EVP of size 128^{10}. $p = 1$, final ranks 8

Newton potential: 11 eigenvalues



$\Omega = (-1,1)^{10}, n = 128 \ \rightarrow$ EVP of size 128^{10}. $p = 11$,
final ranks 40 (cut-off)

Numerical experiments

Henon-Heiles potential:

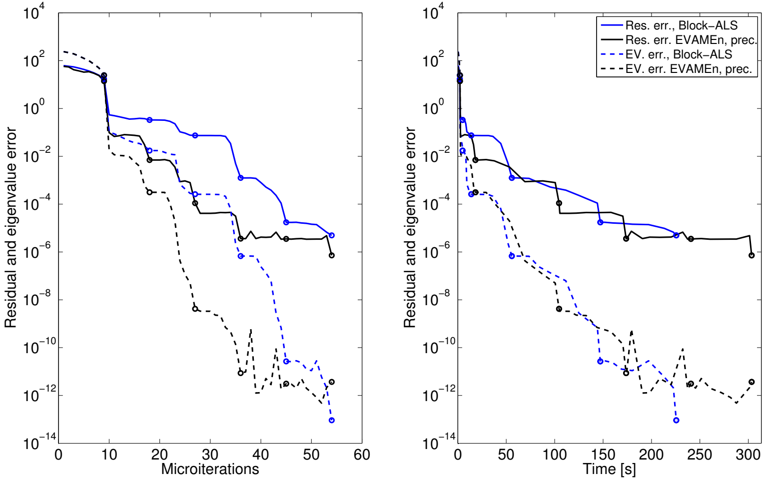
$$V(\mathbf{x}) = \frac{1}{2}\sum_{\mu=1}^{d} x_\mu^2 + \sum_{\mu=1}^{d-1}\left(\sigma_*\left(x_\mu x_{\mu+1}^2 - \frac{1}{3}x_\mu^3\right) + \frac{\sigma_*^2}{16}\left(x_\mu^2 + x_{\mu+1}^2\right)^2\right),$$

modelling a coupled oscillator in quantum physics.

This potential is usually defined on the entire real space. As in [Dolgov et al. 2013] , we apply **spectral collocation**, using a tensor product grid based on the zeros $\xi_1, \ldots, \xi_n$ of the nth Hermite polynomial.

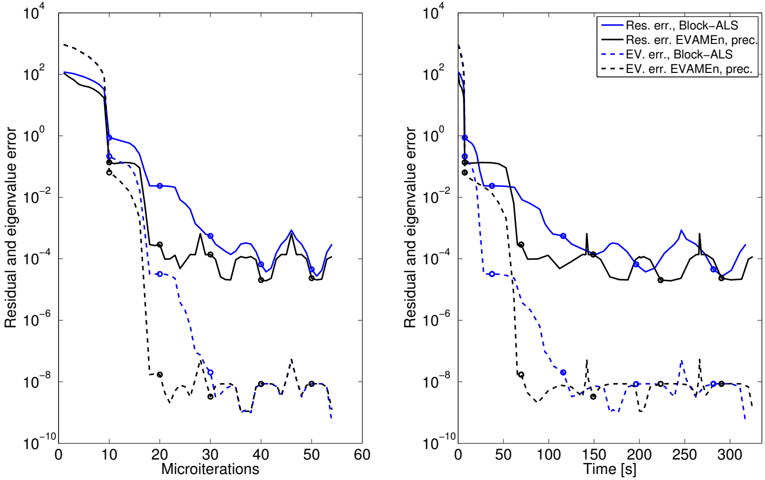
Here: $n = 28$ collocation points in every dimension.

Henon-Heiles potential: 3 eigenvalues



$d = 10, n = 28 \;\rightarrow\;$ EVP of size 28^{10}. $p = 3$

Henon-Heiles potential: 11 eigenvalues



$d = 10, n = 28 \;\rightarrow\;$ EVP of size 28^{10}. $p = 11$

Conclusions

- Tensor techniques, using e.g. the TT format, allow for the solution of extremely high-dimensional eigenvalue problems. Successfully used in physics.
- Need: Low-rank structured operators and low-rank solutions
- (Block)-ALS is extremely efficient and rank-adaptive for $p > 1$
- AMEn injects (preconditioned) residual information to the local problems to speed up convergence and enables rank-adaptivity even for $p = 1$. Reduction in iteration count, but each iteration is more costly.

More details:

D. Kressner, M. Steinlechner, A. Uschmajew:
Low-rank tensor methods with subspace correction for symmetric eigenvalue problems
MATHICSE Technical Report 40.2013, December 2013.
Accepted for publication in SIAM Journal on Scientific Computing.
Available at http://anchp.epfl.ch/publications

Thank you for your attention!