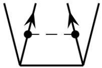
Tensor decomposition methods for high-precision relativistic modeling of electronic structure

Rumyantsev A.S.[1],
Oleynichenko A.V.[1,3], Zaitsevskii A.V.[1,2]

[1] NRC «Kurchatov Institute» - PNPI,
[2] M.V. Lomonosov MSU,
[3] MIPT

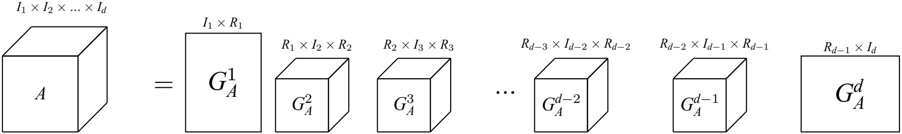
Introduction. CC equations

CCSD		$\sum t_{ij}^{cd} \langle ab \| \| cd \rangle$	$\Rightarrow$	$O(N^6)$
CCSDT		$\sum t_{ijk}^{dec} \langle ab \| \| de \rangle$	$\Rightarrow$	$O(N^8)$
CCSDTQ		$\sum t_{ijkl}^{efcd} \langle ab \| \| ef \rangle$	$\Rightarrow$	$O(N^{10})$

Tensor Train

Tensor A is presented in TT format if

$$A_{i_1 i_2 \dots i_d} = \sum_{\alpha_1 \dots \alpha_d}^{R_1 \dots R_d} G_1[1, i_1, \alpha_1] G_2[\alpha_1, i_2, \alpha_2] \dots G_d[\alpha_d, i_d, 1], \text{ где } G_j \in \mathbb{C}^{R_j \times I_j \times R_{j+1}}$$

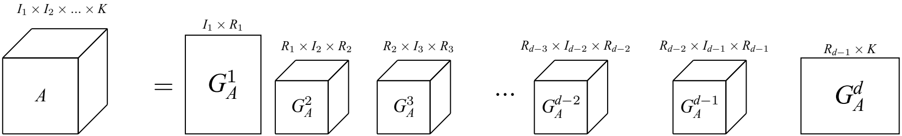


Terminology:

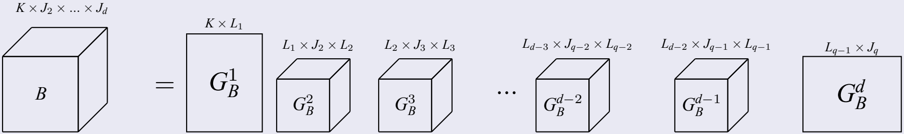
- G_i - TT-core;
- R_i - TT-dimensions;
- $R = \max_i(R_i)$ - maximum TT-dimension.

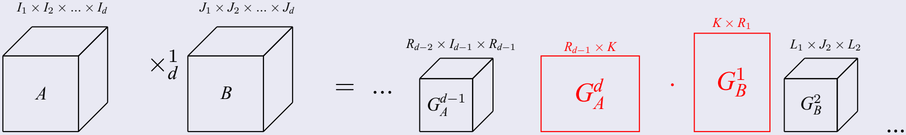
Oseledets I. V. Tensor-Train Decomposition // SIAM Journal on Scientific Computing. 2011. V.33, no. 5. PP. 2295–2317. doi: 10.1137/090752286.

Contraction. TT-TT

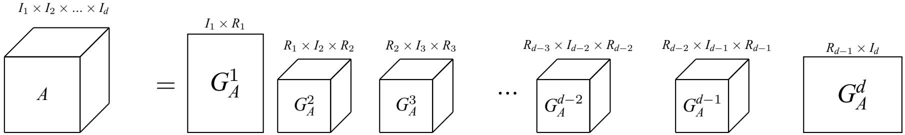


TT-TT

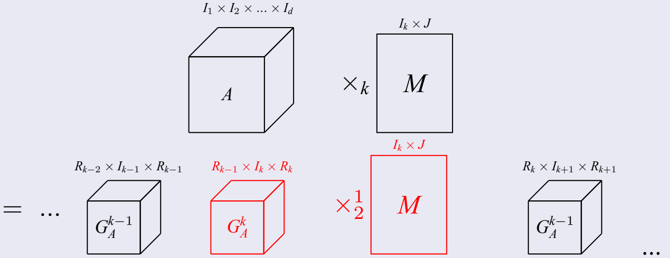




Contraction. TT-Matrix



TT-Матрица



Some conclusions

Advantages

- The complexity of contractions is greatly reduced and, most importantly, depends on the dimension of the tensor linearly;
- Data is being compressed.

Disadvantages

- ”The tensor must be singular”;
- The addition operation increases the size of the cores.

Applications

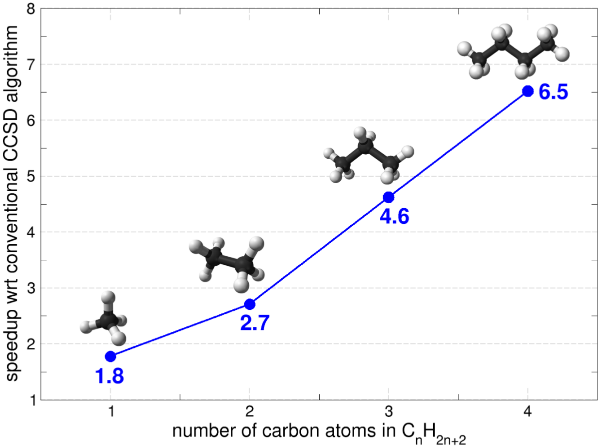


Figure 1: Speeding up the calculation of alkanes

Conclusion

- The library is written in the Rust language and includes functions and decompositions.
- The CCSD approximation is implemented in terms of tensor trains and is almost embedded in the EXP-T software package.
- Implementation of the solution of the CCSDT and CCSDTQ equations in terms of tensor trains.

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Summation. Additionally

A and B are given in TT format:

$$A = G_1^A \times_3^1 G_2^A \times_3^1 \ldots \times_3^1 G_d^A$$
$$B = G_1^B \times_3^1 G_2^B \times_3^1 \ldots \times_3^1 G_d^B$$

It is necessary to find

$$C = A + B.$$

Then the cores for C are defined as follows:

$$G_i^C = \begin{bmatrix} G_i^A & 0 \\ 0 & G_i^B \end{bmatrix}, \text{ для } i = 1, \ldots, d.$$

Thus, C in TT format will look like this:

$$C = G_1^C \times_3^1 G_2^C \times_3^1 \ldots \times_3^1 G_d^C$$