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Tensor Decomposition in Electronic Structure Calculations on 3D Cartesian Grids

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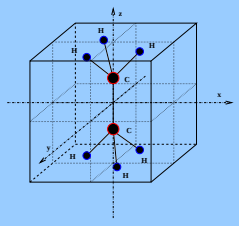


Introduction

Modern problems of physical chemistry lead to computations of many-particle potentials and related integral transforms, involving quantities described by higher-order tensors. Conventional numerical treatment of these problems suffers from the so-called "curse of dimensionality". Recently developed Tucker and canonical tensor approximation techniques provide structured data-sparse representation to higher-order tensors. We discuss the newly developed algorithms of *multi-linear algebra* (MLA) for the numerical treatment of multi-dimensional operators and functions. Applications to the electron density and to the Hartree potential in the Hartree-Fock equation are presented.

Tucker and canonical (CP) tensor approximations in $\mathbb{R}^d$

We approximate the *d-th order tensors* (function of discrete variables)

$$\mathcal{A} = [a_{i_1 \dots i_d}] \in \mathbb{R}^{n^{\otimes d}}, \ i_\ell = 1, \dots, n, \ \ell = 1, \dots, d, \ n \in \mathbb{N}; \quad S(\mathcal{A}) = n^d,$$

by the short-term sum of rank-1 tensors.

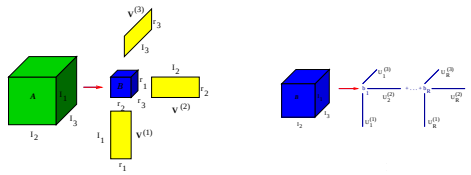
CP model: using a sum of normalized rank-1 tensors

$$\mathcal{A}_{(R)} = \sum_{k=1}^{R} b_k \, U_k^{(1)} \otimes \dots \otimes U_k^{(d)} \approx \mathcal{A}.$$

Tucker model: using orthonormalized set $\{V_{k_\ell}^{(\ell)} \in \mathbb{R}^n, \ k_\ell = 1, \dots, r\}$,

$$\mathcal{A}_{(\mathbf{r})} = \sum_{k_1=1}^{r} \dots \sum_{k_d=1}^{r} b_{k_1 \dots k_d} V_{k_1}^{(1)} \otimes \dots \otimes V_{k_d}^{(d)} \approx \mathcal{A}.$$

Core tensor $\mathcal{B} = \{b_{\mathbf{k}}\} \in \mathbb{R}^{r^{\otimes d}}$ is unique up to rotation, $\|\mathcal{A}_{(\mathbf{r})}\| = \|\mathcal{B}\|$.
In our applications $r \ll R$ and $r \ll n$.
We apply the two-level tensor approximation scheme:



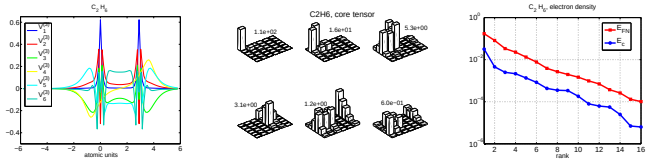
Tucker decomposition (left), CP decomposition (right).

Breaking down the complexity

1. $S(\mathcal{A}_{(R)}) = Rdn + R, \quad S(\mathcal{A}_{(\mathbf{r})}) = rdn + r^d.$
2. Exponential convergence of the tensor approximation upon the Tucker rank

$$E_{FN}^{(r)} = \frac{\|\mathcal{A} - \mathcal{A}_{(r)}\|}{\|\mathcal{A}\|} \lesssim e^{-qr}.$$

3. Almost uniform convergence rate q in the univariate problem size n.
4. Low complexity of MLA operations: storage, inner/outer products, multiplication and convolution product of tensors.



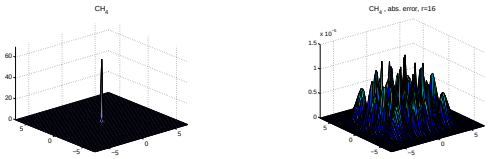
Orthogonal components $V_1^{(3)}, \dots, V_6^{(3)}$ (left), slices of the core tensor for the decomposition with $r = 6$ (middle) and the convergence history upon the Tucker rank for the electron density of C_2H_6 molecule.

Application to electronic structure calculations

The Hartree-Fock equation for the N-electron system is a self-consistent eigenvalue problem in $L^2(\mathbb{R}^3)$

$$\left(-\frac{\Delta}{2} - V_{nucl} + \int_{\mathbb{R}^3} \frac{\rho(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} d\mathbf{y}\right) \phi_i(\mathbf{x}) - \int_{\mathbb{R}^3} \frac{\rho(\mathbf{x},\mathbf{y})\phi_i(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} d\mathbf{y} = \lambda_i \phi_i(\mathbf{x})$$

for $i = 1, \dots, N/2$, with the electron density $\rho(\mathbf{x}) = 2 \sum_{i=1}^{N/2} |\phi_i(\mathbf{x})|^2$.



Electron density of CH_4 molecule and absolute error of its rank $r = 16$ Tucker-type approximation.

Our goal is to compute the Coulomb matrix $\{J_{km}\}$ of the Hartree potential, $V_H = \rho * \frac{1}{|x|}$,

$$J_{km} := \int_{\mathbb{R}^3} g_k(\mathbf{x}) g_m(\mathbf{x}) V_H(\mathbf{x}) d\mathbf{x}, \quad k, m = 1, \dots, R_0,$$

where $\{g_k\}$ represents the GTO basis set.

Using tensor-product convolution

The convolution product is defined by

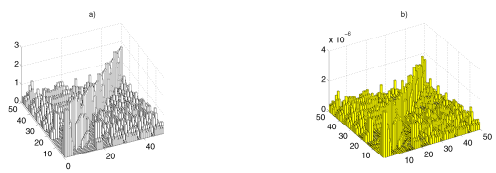
$$(f * g)(x) := \int_{\mathbb{R}^3} f(y) g(x-y) dy \quad f, g \in L^2(\mathbb{R}^3).$$

In our case $g(x) = \frac{1}{|x|}$, $f(x) = \rho(x), x \in \mathbb{R}^3$.
$f * g$ is computed in a fixed box $\Omega = [-A, A]^3$ and f has its support in Ω.

We descretise convolving functions f and g by the collocation scheme on the uniform $n \times n \times n$ tensor-product grid. $\mathcal{F} \in \mathbb{R}^{n^{\otimes 3}}$ is presented in the Tucker/CP format and $\mathcal{G} \in \mathbb{R}^{n^{\otimes 3}}$ is approximated by the rank-R CP tensor using *sinc*-quadratures. The convolution in tensor-product format reads as

$$\mathcal{F} * \mathcal{G} = \sum_{k=1}^{R_1} \sum_{m=1}^{R} c_k b_m \left(V_k^{(1)} * U_m^{(1)}\right) \otimes \dots \otimes \left(V_k^{(3)} * U_m^{(3)}\right),$$

which leads to the cost $\mathcal{N}_{C*C} = O(RR_1 n \log n) \ll O(n^3 \log n)$, where the latter corresponds to 3D FFT.



a) Coulomb matrix for CH_4, b) the absolute error of computations via the tensor approximation.

References

B.N. Khoromskij and V. Khoromskaia, *Low Rank Tucker Tensor Approximation to the Classical Potentials.* Central European J. of Math., 5(3) (2007), 1-28.

B. N. Khoromskij, S.R. Chinnamsetty, H.-J. Flad and V. Khoromskaia. *Tensor Decomposition in Electronic Structure Calculations on 3D Cartesian Grids.* Preprint 65, MPI MIS Leipzig, 2007; J. Comp. Phys. (submitted).

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