Abstract. We propose new cross-conv algorithm for approximate computation of convolution in different low-rank tensor formats (tensor train, Tucker, Hierarchical Tucker). It has better complexity with respect to the tensor rank than previous approaches. The new algorithm has a high potential impact in different applications. The key idea is based on applying cross approximation in the “frequency domain”, where convolution becomes a simple elementwise product. We illustrate efficiency of our algorithm by computing the three-dimensional Newton potential and by presenting preliminary results for solution of the Hartree-Fock equation on tensor-product grids.

Key words. multidimensional convolution, tensor train, tensor decompositions, multilinear algebra, cross approximation, black box approximation

AMS subject classifications. 15A69, 15B05, 44A35, 65F99

1. Introduction. Multivariate convolution problem arises in a range of applications, such as population balance models [7], Smoluchowski equation [60, 50], modeling of quantum mechanical systems with the help of Hartree-Fock and Kohn-Sham equations [4, 63, 26, 27]. Several applications can be found in signal/data processing [62] or even in financial mathematics [40].

The convolution of \( f, g : \mathbb{R}^d \rightarrow \mathbb{R} \) is defined by the integral transform

\[
(f * g)(x) \equiv \int_{\mathbb{R}^d} f(y) g(x - y) \, dy, \quad x \in \mathbb{R}^d.
\]  

(1.1)

We get a discrete convolution problem by a suitable discretization of (1.1) on a uniform grid:

\[
(f * g)_i = \sum_j f_j g_{i-j},
\]  

(1.2)

where \( i, j \in \{0, \ldots, n-1\}^d \) are multi-indices. Usage of uniform grids is typical, but non-obligatory. Non-uniform grids [18, 19] can be used. In this paper we consider only uniform grids and the discrete convolution (1.2) is the main object of study in this paper.

Classic approach to compute the discrete convolution is based on the Fast Fourier Transform (FFT). It requires \( O(n^d \log n) \) operations for a grid with \( n^d \) points. This is much faster than the naive approach (with complexity \( O(n^{2d}) \)), but still prohibitive for large \( d \) and/or \( n \). To reduce computational complexity certain low-parametric representations of \( f \) and \( g \) have to be used. For this task we will use tensor formats which are based on the idea of separation of variables. The most straightforward way to separate variables is to use the canonical polyadic format (CP format, also called...
CANDECOMP/PARAFAC model) which dates back to 1927 [24]. A tensor is said to be in canonical format if it can be represented in the form

\[ A(i_1, \ldots, i_d) = \sum_{\alpha=1}^{r} U_1(i_1, \alpha) \cdots U_d(i_d, \alpha), \]

where the minimal possible \( r \) is called **canonical rank**. If a good CP approximation is known, many basic operations are fast to compute [5, 31, 21, 22, 35, 46, 6].

Nevertheless, the CP decomposition suffers from a serious drawback: there are no robust algorithms to compute it numerically for \( d > 2 \) [10]. Note that in two dimensions it can be computed in a stable way by using SVD or, if the matrix is large, by rank-revealing algorithms.

The Tucker format [57, 8, 9, 35] is another classic decomposition of tensors. It can be computed via stable algorithms but the number of parameters grows exponentially in \( d \). As a result, it is typically used only for problems with small \( d \), especially for the three-dimensional case. In higher dimensions other **stable tensor formats**, namely tensor train (TT) [47, 43] or hierarchical Tucker (HT) [23, 15] formats can be used. In contrast with the Tucker format, they do not suffer from the “curse of dimensionality”. For more details regarding low-rank representations of tensors see the book by Hackbusch [20] and reviews [34, 17, 39].

**Related work.** In this paper we focus on fast computation of multidimensional convolution. Although it is not difficult to implement convolution in complexity linear in \( d \) or \( n \), a strong rank dependence may occur. The rank of the result is generally equal to the product of the ranks of \( f \), \( g \), and then one should truncate the representation with necessary accuracy (by truncation we mean approximation in the same format with smaller rank). This approach was considered in [54, 32] and may lead to high complexity when the ranks are large. A remarkable work is [25] where an algorithm for the computation of convolution in so-called Quantized TT (QTT) [33, 41] was proposed. This algorithm has complexity \( O(d \log^2 n) \) and is asymptotically the best one. However, for \( n \) of practical interest the algorithm proposed in this paper is faster. This is due to high constant hidden in \( O(\cdot) \) term in the QTT algorithm.

The algorithm proposed in this paper is simple. At first, we use a classic idea of representing discrete convolution in the form of several Fourier transforms and one element-wise multiplication in the “frequency domain”. The crucial step is to interpolate this element-wise product via **cross approximation method**. One of the nice properties of the stable (SVD-based) tensor formats (Tucker, TT, HT) is that for each of them there is an algorithm, that allows to accurately reconstruct a low-rank tensor using only few of its elements. The Fourier transform steps do not change the tensor structure, and the element-wise multiplication is done via the cross approximation algorithm.

Our paper is organized as follows. In Section 2 we give a brief summary of notations. In Section 3 we discuss different discretizations that lead to the discrete convolution. The cross-conv algorithm is described in Section 4 and its complexity is analyzed. In Section 5 numerical experiments are presented: we compute three-dimensional Newton potentials of different electronic densities. We also compare our algorithm with one in [25]. Finally, we present preliminary results for the solution of the Hartree-Fock equation on tensor-product grids.

**2. Notation and prerequisites.** In this section we will give a brief summary of notations that we use.
Vectors are just multidimensional arrays. They will be denoted by boldface letters, i.e. $\mathbf{A}$. We denote an element of $\mathbf{A}$ in position $(i_1, \ldots, i_d)$ as $A(i_1, \ldots, i_d)$. The number of indices $d$ will be called dimension of a tensor. Indices $i_k$ vary from 0 to $n_k - 1$ (this makes the notation for the convolution simpler), where $n_k$ are called mode sizes. The Frobenius norm of a tensor is defined as

$$\|\mathbf{A}\| = \sqrt{\sum_{i_1, \ldots, i_d} |A(i_1, \ldots, i_d)|^2}.$$ 

The element-wise tensor multiplication of tensors $\mathbf{A}$ and $\mathbf{B}$ is denoted by $\mathbf{C} = \mathbf{A} \odot \mathbf{B}$ and is defined as

$$C(i_1, \ldots, i_d) = A(i_1, \ldots, i_d)B(i_1, \ldots, i_d).$$

A tensor $\mathbf{A}$ is said to be in the Tucker format [57], if it is represented as

$$A(i_1, \ldots, i_d) = \sum_{\alpha_1, \ldots, \alpha_d} G^{(A)}(\alpha_1, \ldots, \alpha_d)U_1^{(A)}(i_1, \alpha_1) \cdots U_d^{(A)}(i_d, \alpha_d),$$

where $\alpha_k$ varies from 1 to $r_k$. The minimal number of summands $r_k$ required to represent $\mathbf{A}$ in the form (2.1) is called the Tucker rank of $k$-th mode. The tensor $G^{(A)}$ is called the core of the decomposition and $U_k^{(A)}$ are referred to as Tucker factors. The Tucker decomposition contains $O(r^d + nr^d)$ elements, so the number of parameters grows exponentially in $d$.

Tensor train (TT) (or MPS in other communities) and Hierarchical Tucker (HT) formats are efficient low-parametric representations of multidimensional tensors. A tensor $\mathbf{A}$ is said to be in the TT-format [47, 43] if it can be written in the form

$$A(i_1, \ldots, i_d) = \sum_{\alpha_0, \ldots, \alpha_d} G_1^{(A)}(\alpha_0, i_1, \alpha_1)G_2^{(A)}(\alpha_1, i_2, \alpha_2) \cdots G_d^{(A)}(\alpha_{d-1}, i_d, \alpha_d).$$

(2.2)

In (2.2) $G_k$ have sizes $r_{k-1} \times n_k \times r_k$ and are called TT-cores, where $r_0 = 1$ and $r_d = 1$. The numbers $r_k$ are called TT-ranks of the representation. The decomposition (2.2) can be also written in the matrix-product form (Matrix Product State, MPS)

$$A(i_1, \ldots, i_d) = G_1^{(A)}(i_1)G_2^{(A)}(i_2) \cdots G_d^{(A)}(i_d),$$

where $G_k(i_k)$ are $r_{k-1} \times r_k$ matrices that depend on parameter $i_k$. It is worth to note that the MPS representation, which is algebraically equivalent to the TT-format, has been used for a long time in quantum information theory and solid state physics to approximate certain wavefunctions [61, 49], see the review [56] for more details.

Discrete Fourier Transform is crucially required for fast convolution algorithms. We denote by $\mathcal{F}(\mathbf{A})$ Fourier transform of the tensor $\mathbf{A}$:

$$\mathcal{F}(\mathbf{A})(i_1, \ldots, i_d) = \sum_{j_1, \ldots, j_d} e^{-2\pi i \left( \frac{i_1 j_1}{n_1} + \cdots + \frac{i_d j_d}{n_d} \right)} A(j_1, \ldots, j_d),$$

and by $\mathcal{F}^{-1}(\mathbf{A})$ inverse Fourier transform:

$$\mathcal{F}^{-1}(\mathbf{A})(i_1, \ldots, i_d) = \frac{1}{n_1 \cdots n_d} \sum_{j_1, \ldots, j_d} e^{2\pi i \left( \frac{i_1 j_1}{n_1} + \cdots + \frac{i_d j_d}{n_d} \right)} A(j_1, \ldots, j_d).$$
### 3. Discretization

For convenience we describe here well-known facts about the discretization of the convolution, see, for example, [32]. Recall that the multidimensional convolution of \( f, g : \mathbb{R}^d \to \mathbb{R} \) is defined by the integral transform

\[
(f \ast g)(x) \equiv \int_{\mathbb{R}^d} f(y)g(x - y) \, dy, \quad x \in \mathbb{R}^d.
\]

We assume that \( f \) is small enough outside some cube \( \Omega = [-L, L]^d \) so that we can replace the domain of integration by \( \Omega \). The size of the box depends on the application, but many applications (like electronic structure computation) involve functions that decay exponentially with \( \|x\| \to \infty \) and the selection is obvious. There are three standard methods to discretize convolutions: Galerkin method, collocation method and Nyström-type schemes.

First, introduce in \( \Omega \) a uniform tensor-product grid \( \omega^h = \omega^h_1 \times \cdots \times \omega^h_d \) with \( h = 2L/n \), where \( \omega^h_i = \{-L + kh : k = 0, \ldots, n\}, i = 1, \ldots, d \). For simplicity, consider piecewise-constant basis functions \( \phi_i \) with support on \( \Omega_i \), where \( i \in \mathcal{I} \equiv \{0, \ldots, n-1\}^d \) and \( \Omega_i \) are \( h^d \) cubes centered in \( y_i \). Thus, we have

\[
(f \ast g)(x) \approx \sum_{i \in \mathcal{I}} f_i \int_{\Omega_i} \phi_i(y)g(x - y) \, dy,
\]

where \( f_i \) are the coefficients in the expansion \( f(y) \approx \sum_{i \in \mathcal{I}} f_i \phi_i(y) \). As a result, the collocation scheme with collocation points \( x_j \) yields a discrete convolution:

\[
w_j \equiv (f \ast g)(x_j) \approx \sum_i f_i g_{i-j}, \quad j \in \mathcal{I},
\]

where

\[
g_{i-j} = \int_{\Omega_i} \phi_i(y)g(x_j - y) \, dy,
\]

is a multilevel Toeplitz matrix. The problem with the collocation method is that it leads to non-symmetric Toeplitz matrices even if the original convolution was symmetric. This may pose problems in some applications. A natural choice is to use a Galerkin method, which again leads to the discrete convolution with

\[
g_{i-j} = \int_{\mathbb{R}^d} \phi_i(x)\phi_j(y)g(x - y) \, dx \, dy, \quad f_i = \int_{\mathbb{R}^d} f(x)\phi_i(x) \, dx.
\]

To get high-order discretization schemes translation-invariant basis-functions of higher order can be used \( \phi_i(y) = \psi(y - y_i) \), where \( \psi(y) \) is a suitable piecewise-polynomial function. Computation of matrix elements in (3.3) or (3.4) even for piecewise-constant functions can be complicated. A simple alternative is a Nyström-type scheme that uses shifted grids [11]

\[
(f \ast g)(x_j) \approx h^d \sum_{i \in \mathcal{I}} f(y_i)g(x_j - y_i), \quad j \in \mathcal{I},
\]

where \( x_j \) are points of \( y_i \) shifted by half step. For a certain class of functions it provides almost second order of accuracy up to a logarithmic term.
4. **Algorithm description.** Let us consider a $d$-dimensional discrete convolution of two tensors $f_i$ and $g_j$

$$w_j = \sum_{i \in I} f_i g_{i-j}, \quad j \in I. \tag{4.1}$$

This can be also considered as a product of *multilevel Toeplitz matrix* with elements $g_{i-j}$ by a vector (see, for example, [58] for properties of multilevel Toeplitz matrices). The computation of (4.1) as a direct sum requires $O(n^{2d})$ operations. Using the FFT the complexity can be reduced to $O(n^d \log n)$. The classic FFT-based algorithm is our starting point for an efficient low-rank convolution algorithm.

The idea of the FFT method is to replace a Toeplitz matrix by vector product to a product of a larger *circulant* matrix by a vector. For instance, a 1-level $n \times n$ Toeplitz matrix $\{g_{i-j}\}_{i,j=0}^{n-1}$ may be embedded in an $(2n-1) \times (2n-1)$ circulant matrix which is fully defined by its first column $c_g \equiv \{g_0, g_1, \ldots, g_{n-1}, g_{1-n}, g_{2-n}, \ldots, g_{-1}\}$.

In the $d$-dimensional case a multilevel circulant matrix is defined by a tensor $c_g$:

$$c_g(i_1, \ldots, i_d) = g_{\tau(i_1), \ldots, \tau(i_d)}, \quad i_1, \ldots, i_d \in [0, 2n-2],$$

where

$$\tau(i) = \begin{cases} i, & i \in [0, n-1], \\ i - 2n + 1, & i \in [n, 2n-2]. \end{cases}$$

At the first step we embed $f$ into a larger tensor $q_f$ with mode sizes $(2n_1-1, \ldots, 2n_d-1)$ by zero-padding:

$$q_f(i_1, \ldots, i_d) = \begin{cases} f_{i_1, \ldots, i_d}, & i_1, \ldots, i_d \in [0, n-1], \\ 0, & \text{otherwise}. \end{cases}$$

Multilevel circulant matrices are diagonalized by the normalized unitary Fourier matrix $\frac{1}{n^{d/2}} F_d$ and the eigenvalues can be computed from the DFT of the first column,

$$C = \frac{1}{n^d} F_d^* \Lambda F_d,$$

where

$$\Lambda = \text{diag}(\mathcal{F}(c_g)).$$

Therefore,

$$\tilde{w} = F^{-1}(\mathcal{F}(c_g) \circ \mathcal{F}(q_f)), \tag{4.2}$$

where $\tilde{w}$ is the expanded convolution tensor with $(2n-1)$ each mode size and we are interested only in its subtensor $w$:

$$w(i_1, \ldots, i_d) = \tilde{w}(i_1, \ldots, i_d), \quad i_1, \ldots, i_d \in [0, n-1].$$

How to use this formula if the operands are given in a low-rank tensor format? For simplicity, consider that $c_g$ and $q_f$ are in the TT-format

$$c_g(i_1, \ldots, i_d) = G_1^{(c_g)}(i_1) \ldots G_d^{(c_g)}(i_d),$$

$$q_f(i_1, \ldots, i_d) = G_1^{(q_f)}(i_1) \ldots G_d^{(q_f)}(i_d), \tag{4.3}$$
however the idea applies to other SVD-based formats (Tucker, HT, skeleton). The Fourier matrix has a tensor product structure: 

\[ F_d = F \otimes F \otimes \ldots \otimes F, \]

therefore, its application does not change the TT-ranks (as well as the inverse Fourier transform). Indeed, given a tensor \( A \) in the TT-format, the \( F(A) \) can be written in the following form:

\[
F(A)(i_1, \ldots, i_d) = \sum_{j_1, \ldots, j_d} e^{-2\pi i \left[ \frac{i_1 j_1}{a_1} + \cdots + \frac{i_d j_d}{a_d} \right]} G_1(A)(j_1) \ldots G_d(A)(j_d) = \\
= \sum_{j_1} e^{-2\pi i \frac{i_1 j_1}{a_1}} G_1(A)(j_1) \ldots \sum_{j_d} e^{-2\pi i \frac{i_d j_d}{a_d}} G_d(A)(j_d) = \\
= F_{1D} \left( G_1^A \right)(i_1) \ldots F_{1D} \left( G_d^A \right)(i_d),
\]

where by \( F_{1D} \) we denote a 1-dimensional Fourier transform.

Now we are ready to describe the algorithm.

**Step 1.** Compute tensors \( F(c_g) \) and \( F(q_f) \) in the considered format. As was mentioned above, Fourier transform of any tensor does not change its ranks and is equivalent to univariate Fourier transforms of each factor in the Tucker case and each core in the TT case. Therefore in the TT-format,

\[
F(c_g)(i_1, \ldots, i_d) = F_{1D} \left( G_1^{c_g} \right)(i_1) \ldots F_{1D} \left( G_d^{c_g} \right)(i_d),
\]

\[
F(q_f)(i_1, \ldots, i_d) = F_{1D} \left( G_1^{q_f} \right)(i_1) \ldots F_{1D} \left( G_d^{q_f} \right)(i_d),
\]

**Step 2.** In this step we compute element-wise product \( \Theta = F(c_g) \circ F(q_f) \) and this is the crucial step of our algorithm. The naive approach is to compute it directly and it leads to the tensor representation with the ranks squared. The truncation is almost always required, and for the TT-format it leads to an algorithm with complexity \( O(dnR^3) \), where \( R = r^2 \). Such algorithm works only up to ranks \( r_k \approx 100 \). There are more sophisticated algorithms for different formats that are based on iterative schemes, e.g. for Tucker [14, 55] and for TT-format [42, 12], but they work on the resulting tensor. We propose to compute the element-wise product via sampling. It is very cheap to compute any prescribed element of the product, and that situation is perfectly suited for the application of cross approximation methods. Such methods are proposed for all of the SVD-based formats and require the same amount of elements to be sampled, as the number of parameters in the decomposition! We will give corresponding complexity estimates in the next section. Thus, we compute necessary elements of the tensors \( F(c_g) \) and \( F(q_f) \), multiply them and build a tensor \( \Theta \) in the considered format according to those elements and selected cross approximation scheme. This is the only step where approximation is done. Suppose that the approximation error is \( \delta \):

\[
\Theta(i_1, \ldots, i_d) = \tilde{\Theta} + \Delta \Theta,
\]

where

\[
\tilde{\Theta}(i_1, \ldots, i_d) = G_1^{(\Theta)}(i_1) \ldots G_d^{(\Theta)}(i_d),
\]

is the approximation of \( \Theta \) computed via a cross method with relative accuracy \( \|\Delta \Theta\|/\|\Theta\| = \delta \).
Step 3. Compute $F_{1D}^{-1}$ of each $\Theta$ core. Therefore, the final approximation $\tilde{w}$ has the form

$$\tilde{w} = F^{-1}(\Theta)(i_1, \ldots, i_d) = F_{1D}^{-1} \left( G_{1}^{(\Theta)} \right)(i_1) \ldots F_{1D}^{-1} \left( G_{d}^{(\Theta)} \right)(i_d) + F^{-1}(\Delta \Theta).$$

It is easy to estimate the required threshold $\delta$ to be provided to the cross approximation algorithm. Suppose $\epsilon = \|\Delta \tilde{w}\|/\|\tilde{w}\|$, is the required accuracy, where $\Delta \tilde{w} = F^{-1}(\Delta \Theta)$. Due to unitary invariance of the Frobenius norm we have

$$\epsilon = \frac{\|\Delta \tilde{w}\|}{\|\tilde{w}\|} = \frac{\|F^{-1}(\Delta \Theta)\|}{\|F^{-1}(\Theta)\|} = \frac{\|\Delta \Theta\|}{\|\Theta\|} = \delta.$$

So, to provide the convolution accuracy $\epsilon$ one needs to run the cross approximation algorithm with $\delta(\epsilon) = \epsilon$.

4.1. Algorithm complexity in different formats. Let us estimate the complexity for different formats. For simplicity, in the complexity estimates we assume that tensors $c_g$, $q_f$ and $\tilde{w}$ have $n_k \sim n$ and $r_k \sim r$. Our additional assumption in the complexity estimates is that the result of the convolution can be well approximated with the ranks $R_k \ll r^2$. This assumption has to be verified for each particular case, but it is standard for such kind of algorithms.

Skeleton decomposition. First, consider two-dimensional case. In two dimensions the only way to separate variables is to approximate a matrix $A \in \mathbb{C}^{n \times m}$ by a skeleton decomposition:

$$A \approx UV^T,$$

where $U \in \mathbb{C}^{n \times r}$, $V \in \mathbb{C}^{m \times r}$ and $r$ is an approximate rank of the matrix $A$. Cross algorithms to compute the skeleton decomposition require $r$ columns and $r$ rows to be computed. Computation of a column or a row of a matrix given by its skeleton decomposition costs $O(nr)$ operations. Indeed, consider the computation of the $j$-th column:

$$A(:, j) = UV(j, :)^T.$$

The computation of the product $UV(j, :)^T$ requires $nr$ operations. As a result, the evaluation of $r$ crosses of the matrix $\Theta = F(c_g) \circ F(q_f)$ from step 2 needs $O(nr^2)$ flops. Additional operations performed in the cross approximation methods also have $O(nr^2)$ complexity [59, 2]. Note, that the FFT operations from steps 1 and 3 cost $O(rn \log n)$ operations. Thus, the algorithm complexity in the two-dimensional case is $O(nr^2 + rn \log n)$.

Tucker format. The Tucker format contains exponential in $d$ number of parameters $O(r^d + nrd)$, but it can be efficient for problems with small $d$, especially for the case $d = 3$. Let us calculate the complexity of the three-dimensional convolution in the Tucker format. Several implementations of cross-types methods for the Tucker format are available, with the first one (Cross-3D) proposed in [45], see also [36, 3] for other approaches. For the numerical experiments in this paper we implemented a new variant of the Cross-3D method which has better asymptotic complexity in $r$ than the method described in [45]. We will report the details of the implementation in a forthcoming paper. This method requires the computation of fibers (which are three-dimensional generalization of columns and rows). For the interpolation, $r$ fibers
in each direction must be computed. Let us estimate the complexity of such computation, when our approximated tensor is given as an element-wise product of two tensors in the Tucker format. Let tensors \( \mathcal{F}(c_g) \) and \( \mathcal{F}(q_f) \) be in the Tucker format. A fiber is defined by two fixed indices, for example, let \( \mathbf{A} \) be a tensor,

\[
\mathbf{A}(i_1, i_2, i_3) = \sum_{\alpha_1, \alpha_2, \alpha_3} G^{(A)}(\alpha_1, \alpha_2, \alpha_3) U_1^{(A)}(i_1, \alpha_1) U_2^{(A)}(i_2, \alpha_2) U_3^{(A)}(i_3, \alpha_3),
\]

and \( i_2, i_3 \) are the fixed indices (and we need to compute the result for all \( i_1 = 0, \ldots, n-1 \)). First, we calculate

\[
B_{i_2 i_3}(\alpha_1) = \sum_{\alpha_2, \alpha_3} G^{(A)}(\alpha_1, \alpha_2, \alpha_3) U_2^{(A)}(i_2, \alpha_2) U_3^{(A)}(i_3, \alpha_3),
\]

and this step requires \( O(r^3) \) operations. Then a first mode fiber is

\[
\mathbf{A}(\cdot, i_2, i_3) = \sum_{\alpha_1} U_1^{(A)}(\cdot, \alpha_1) B_{i_2 i_3}(\alpha_1),
\]

and that step requires \( O(nr) \) operations. Thus, the computation of one fiber of \( \mathbf{\Theta} = \mathcal{F}(c_g) \circ \mathcal{F}(q_f) \) costs \( O(nr + r^3) \) flops. Since the Cross-3D method uses \( r \) fibers in each direction, the element-wise product complexity is \( O(nr^2 + r^4) \).

As in two-dimensional case, for a tensor \( \mathbf{A} \) in the Tucker format, the Fourier transform \( \mathcal{F}(\mathbf{A}) \) does not change its Tucker ranks and is equivalent to three one-dimensional FFTs of the Tucker factors. Thus, the complexity of the steps 1 and 3 is \( O(nr \log n) \). The total complexity for the approximate convolution in the Tucker format is \( O(nr^2 + r^2 n \log n) \) and that possibly allows for very large \( n \) and \( d \).

**TT format.** For high dimensions the Tucker format becomes unusable, and the TT-format or HT-format that have linear scaling with \( d \) should be used. A cross method for the TT-format was proposed first in [53] and later significantly improved in [52] (and possible improvements are still on the way!). The asymptotic complexity of those algorithms in our case can be shown to be equal to \( O(dnr^3) \) flops. The algorithm consists in \( d \) multiplications of matrices of size \( r \times r \) by matrices of size \( r \times nr \). The FFT step can be implemented via one-dimensional FFTs of each TT-core and it costs \( O(r^2 n \log n) \) flops. The final algorithm complexity is \( O(dnr^3 + r^2 n \log n) \) and that possibly allows for very large \( n \) and \( d \).

**HT and extended TT formats.** If \( n \) is very large, additional complexity reduction can be achieved by using either HT or extended TT-formats. A variant of the cross method for the HT-format can be found in [1]. HT-format can be considered as a sequential application of the Tucker decomposition, while the extended TT-format uses one preliminary Tucker decomposition and then applies TT-decomposition to the Tucker core. Note that the TT-format can be considered as a special case of the HT-format with a linear reduction tree. However, there is a freedom in the TT-format since it is different for different orderings of the indices. In practice TT-format is often found to be much more simple to work with, however there are examples of tensors where the HT-format gives better approximation [10]. If we assume that all ranks are bounded by \( r \), the complexity of the convolution algorithm will be \( O(dnr^2 + dr^4 + r^2 n \log n) \) flops. Note that it has better complexity with respect to \( n \). The complexity estimates are summarized in the Table 4.1.
### Table 4.1

Cross-conv complexity in different formats

| Format                | Complexity            |
|-----------------------|-----------------------|
| Skeleton decomposition| $O(nr^2 + rn \log n)$ |
| Tucker 3D             | $O(nr^2 + r^4 + rn \log n)$ |
| TT                    | $O(dnr^3 + r^2n \log n)$ |
| HT/extended TT        | $O(dnr^2 + dr^4 + rn \log n)$ |

5. **Numerical experiments.** In the numerical experiments we consider a three-dimensional case and the Tucker format. We use a new implementation of the Cross-3D approximation algorithm. Cross-3D and cross-conv algorithms are implemented in Python. Their implementation and the toolbox of basic tensor operations can be found at [https://github.com/rakhuba/tucker3d](https://github.com/rakhuba/tucker3d). The version of numerical experiments described in this paper can be found at [https://bitbucket.org/rakhuba/crossconv-experiment](https://bitbucket.org/rakhuba/crossconv-experiment). Molecule data is provided as well. For the basic linear algebra tasks the MKL library is used. Python and MKL are from the Enthought Python Distribution (EPD 7.3-1, 64-bit) [https://www.enthought.com](https://www.enthought.com) Python version is 2.7.3. MKL version is 10.3-1. Tests were performed on 4 Intel Core i7 2.6 GHz processor with 8GB of RAM. However, only 2 threads were used (this is default number of threads for MKL). We would like to emphasize that implementation of the whole algorithm is in Python and time performance can be considerably improved by implementing the most time-consuming parts of it in C or Fortran languages.

5.1. **Newton potential in 3D.** As the first example we consider a computation of the Newton potential which is the convolution with $1/r$ in three dimensions

$$V(x) = \left( f \ast \frac{1}{\|\cdot\|} \right)(x) \equiv \int_{\mathbb{R}^3} \frac{f(y)}{\|x - y\|} \, dy,$$

where $x = (x_1, x_2, x_3) \in \mathbb{R}^3$ and $\|x\| = \sqrt{x_1^2 + x_2^2 + x_3^2}$. Convolutions of such type typically arise in electronic structure calculations and serve as a testbed for different low-rank methods. To discretize (5.1) we use a Nyström-type scheme (3.5) on two shifted uniform $n \times n \times n$ grids. The discretization error can be shown to be $O(h^2 |\log h|)$ where $h$ is the mesh size.

**Comparison with QTT matrix-by-vector multiplication.** First we compare our algorithm with the algorithm of [25], based on the matrix-by-vector multiplication in the QTT-format (further QTT algorithm). We used the MATLAB implementation that is available as a part of the TT-Toolbox [44], and also replaced the fast DMRG approximate matrix-by-vector product [42] used in the original article by a more efficient AMEN-based matrix-by-vector product [12] [13]. The complexity of the QTT algorithm is logarithmic in the mode size. However, QTT ranks may be considerably larger than the Tucker ranks. Therefore, there is a mode size interval where the cross-conv algorithm is faster despite the fact it is asymptotically slower. To illustrate this fact we consider the computation of the Newton potential of a Slater function $f(y) = e^{-\zeta |y|}$ with $\zeta = 1$. Figure 5.1 shows the ratio of the computational times as a function of the mode size. The actual timings are given in Table 5.1. It is clear that the more accurate the computations are (or the bigger ranks are), the faster the cross algorithm is with respect to the QTT algorithm. Moreover, it is always faster in a practically interesting range $n \sim 10^3 - 10^4$. 


Fig. 5.1. Ratio of QTT algorithm time to cross algorithm time as a function of $n$.

Table 5.1

| $n / \epsilon$ | $2^7$ | $2^8$ | $2^9$ | $2^{10}$ | $2^{11}$ | $2^{12}$ | $2^{13}$ | $2^{14}$ | $2^{15}$ | $2^{16}$ | $2^{17}$ | $2^{18}$ |
|-----------------|-------|-------|-------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| Cross-conv timing (sec) |       |       |       |           |           |           |           |           |           |           |           |           |
| $10^{-3}$ | 0.03  | 0.04  | 0.063 | 0.12     | 0.2       | 0.5       | 1.0       | 2.2       |           |           |           |           |
| $10^{-7}$ | 0.061 | 0.091 | 0.13  | 0.24     | 0.41      | 1.1       | 2.3       | 5.2       | 11.5      |           |           |           |
| $10^{-9}$ | 0.14  | 0.19  | 0.3   | 0.5      | 0.96      | 2.0       | 4.1       | 8.6       | 17.5      | 35.3      | 70.9      | 142.3     |

| QTT timing (sec) |       |       |       |           |           |           |           |           |           |           |           |           |
| $10^{-3}$ | 0.42  | 0.56  | 0.71  | 0.87     | 1.0       | 1.2       | 1.3       | 1.5       |           |           |           |           |
| $10^{-7}$ | 1.7   | 2.5   | 3.6   | 4.8      | 6.0       | 7.2       | 8.6       | 9.8       | 10.9      |           |           |           |
| $10^{-9}$ | 7.1   | 12.1  | 18.4  | 25.9     | 34.0      | 41.9      | 50.3      | 59.0      | 67.7      | 76.4      | 85.1      | 93.8      |

| 3D FFT timing (sec) |       |       |       |           |           |           |           |           |           |           |           |           |
| $10^{-3}$ |       |       |       |           |           |           |           |           |           |           |           |           |
| $10^{-7}$ | 1.3   | 12.6  | 118.7 | 1120     |           |           |           |           |           |           |           |           |
| $10^{-9}$ |       |       |       |           |           |           |           |           |           |           |           |           |

Newton potential of different molecules. One of the applications of fast computation of the Newton potential are the electronic structure computations, where the function $\rho$ is the electron density. We take precomputed values of $\rho$ in the Tucker format. The one-dimensional mode size is $n = 5121$. The Tucker format representation was computed in [54] and the data was kindly provided to us by Dr. Dmitry Savostyanov. Convolution times for different molecules are presented in Table 5.2.

The local filtration algorithm used in [54] has formal complexity $O(nr^2 + r^5)$ for the convolution of a tensor in the canonical format with a tensor in the Tucker format. For the convolution of two Tucker tensors its complexity is $O(nr^2 + r^6)$ compared with $O(nr^2 + r^4)$ complexity of the cross-conv. We did our own implementation of the Tucker-Tucker case from [54] and found that the Tucker ranks after local filtration are not small. For instance, Tucker ranks of the Newton potential of C$_2$H$_6$ are $361 \times 589 \times 532$ before the filtration and $82 \times 144 \times 140$ after the filtration, while the actual ranks are $19 \times 31 \times 28$. Due to the strong rank dependence this leads to significantly
Timing for the computation of the Newton potential for different molecules on the \( n^3 = 5121^3 \) grid

| Molecule     | Accuracy | \( q_f \) ranks | \( \tilde{w} \) ranks | Time (s) |
|--------------|----------|------------------|------------------------|----------|
| CH\(_4\)     | \( 10^{-7} \) | \( 26 \times 26 \times 26 \) | \( 22 \times 22 \times 22 \) | 1.3      |
|              | \( 10^{-7} \) | \( 39 \times 39 \times 39 \) | \( 39 \times 39 \times 39 \) | 4.1      |
|              | \( 10^{-9} \) | \( 52 \times 52 \times 52 \) | \( 58 \times 58 \times 58 \) | 6.4      |
| C\(_2\)H\(_6\) | \( 10^{-5} \) | \( 19 \times 30 \times 27 \) | \( 15 \times 23 \times 20 \) | 1.2      |
|              | \( 10^{-7} \) | \( 28 \times 49 \times 40 \) | \( 24 \times 42 \times 39 \) | 3.9      |
|              | \( 10^{-9} \) | \( 42 \times 66 \times 57 \) | \( 39 \times 66 \times 60 \) | 6.2      |
| C\(_2\)H\(_5\)OH | \( 10^{-5} \) | \( 43 \times 42 \times 43 \) | \( 28 \times 28 \times 29 \) | 2.3      |
|              | \( 10^{-7} \) | \( 66 \times 67 \times 69 \) | \( 50 \times 50 \times 51 \) | 7.5      |
|              | \( 10^{-9} \) | \( 91 \times 90 \times 94 \) | \( 78 \times 79 \times 81 \) | 19.8     |
| C\(_2\)H\(_5\)NO\(_2\) | \( 10^{-5} \) | \( 24 \times 60 \times 60 \) | \( 15 \times 33 \times 33 \) | 2.6      |
|              | \( 10^{-7} \) | \( 35 \times 93 \times 96 \) | \( 26 \times 61 \times 62 \) | 9.4      |
|              | \( 10^{-9} \) | \( 45 \times 126 \times 133 \) | \( 42 \times 97 \times 100 \) | 18.4     |

Larger computational time: thus, the cross-conv algorithm is more robust than the local filtration algorithm.

5.2. Hartree-Fock equation for systems with one closed shell. Three-dimensional convolution appears a substep in the solution of Hartree-Fock or Kohn-Sham equations in electronic structure computations. This is a classic topic and a lot of software packages are available. Here we report only preliminary results. In a series of papers Khoromskij and Khoromskaia have first used grid-based tensor methods for the solution of the Hartree-Fock equation [30, 26, 37, 27, 38, 29, 28]. However, the methods they proposed are not fully “black-box”, since they still require storage of the global basis functions for the solution, and that introduces a basis set error into the solution. We would like to store the solution of the Hartree-Fock equation as a function on a grid, i.e., as a tensor. Good news is that the solution process can be implemented solely in terms of convolutions. This is a topic of ongoing work, and in this paper we present a preliminary numerical experiment for the simplest possible case. A closed-shell Hartree-Fock equation for atoms or molecules with 2 electrons has the form

\[
\left( -\frac{1}{2} \Delta + V \right) \psi = E \psi, \text{ where } V(x) = -\sum_{\alpha} \frac{Z_{\alpha}}{\|x - R_{\alpha}\|} + \int_{\mathbb{R}^3} \frac{|\psi(y)|^2}{\|x - y\|},
\]

\( Z_{\alpha} \) and \( R_{\alpha} \) are charges and coordinates of nuclei, \( \psi(x) \) is the only unknown spatial orbital with \( x \in \mathbb{R}^3 \) and \( E \) is the Hartree-Fock energy. Instead of the classic self consistent field (SCF) iterations we use the integral iterations (see [4])

\[
\hat{\psi} = -2(\Delta - 2E)^{-1} V \psi \equiv -2(V \psi) \star \frac{e^{-\sqrt{-2E}\|\cdot\|}}{4\pi\|\cdot\|},
\]

(with \( \hat{\psi} \) normalized after each iteration step) where \( E \) is also recomputed at each iteration step as \( \hat{E} = E + \langle \hat{\psi}, V \hat{\psi} - V \psi \rangle / \| \hat{\psi} \|^2 \). Note that \((\Delta - 2E)^{-1}\) is an integral operator which is computed via the convolution with Yukawa kernel. At each iteration arising convolutions with Newton and Yukawa kernels are discretized via the symmetric Galerkin scheme [3,4] with piecewise-constant basis functions. Note again that
the grid-based HF solver does not suffer from the basis set error and one can achieve necessary precision by taking larger and larger grids, i.e. reach the Hartree-Fock limit. Table 5.3 illustrates this fact for the Helium atom. The value of the HF-limit was taken from [51]. On Figure 5.2 pictures of the computed He and H$_2$ densities are presented.

**Table 5.3**

**Helium atom. Dependence of the error in the Hartree-Fock energy from the grid size. $\epsilon = 10^{-6}$**

| $n$ (1024, 2048, 4096) | Extrapolation | HF limit (E) |
|------------------------|---------------|--------------|
| $E_{H}$ (Hartree)      |               | -2.86113     |
| $\frac{|E_{H} - E|}{E}$|               | -2.86152     |
| Time, (s)              |               | -2.86164     |
|                        |               | -2.861682    |
|                        |               | -2.861679    |
|                        | 1.9e-04       | 5.3e-05      |
|                        | 1.25e-05      | 0.96e-06     |
|                        | 3.8           | 7.9          |
|                        | 14.3          | -            |
|                        | -             | -            |

**Fig. 5.2.** He density (left) and H$_2$ density (right)

**6. Conclusion and future work.** We have presented a new efficient cross-conv algorithm for the approximate computation of multidimensional convolution in low-rank tensor formats. The numerical experiments show that it is more efficient than the recently proposed QTT approach in a range of practically interesting mode sizes (up to $n \sim 10^4$), and the gain is higher for higher approximation accuracies or ranks. Further research will include applications of the cross-conv algorithm to a number of practically interesting models such as the Hartree-Fock and Smoluchowski equations.

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