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Boris N. Khoromskij

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$O(d \log N)$-Quantics Approximation of N-d Tensors in High-Dimensional Numerical Modeling

Boris N. Khoromskij
Max-Planck-Institute for Mathematics in the Sciences,
Inselstr. 22-26, D-04103 Leipzig, Germany; {bokh}@mis.mpg.de

Dedicated to Prof. W. Dahmen on the occasion of his 60-th birthday

Abstract

In the present paper, we discuss the novel concept of super-compressed tensor-structured data formats in high dimensional applications. We describe the multi-folding or *quantics* based tensor approximation method of $O(d \log N)$-complexity (logarithmic scaling in the volume size), applied to the discrete functions over the product index set $\{1, ..., N\}^{\otimes d}$, or briefly N-d tensors of size N^d, and to the respective discretised differential-integral operators in $\mathbb{R}^d$. As the basic approximation result, we prove that complex exponential sampled on equispaced grid has quantics rank 1. Moreover, the Chebyshev polynomial sampled over Chebyshev Gauss-Lobatto grid, has separation rank 2 in quantics tensor format, while for the polynomial of degree m the respective quantics rank is at most $m + 1$. For N-d tensors generated by certain analytic functions, we give the constructive proof on the $O(d \log N \log \varepsilon^{-1})$-complexity bound for their approximation by low rank 2-$(d \log N)$ quantics tensors up to the accuracy $\varepsilon > 0$. In the case $\varepsilon = O(N^{-\alpha})$, $\alpha > 0$, our approach leads to the quantics tensor numerical method in dimension d, with the nearly optimal asymptotic complexity $O(d/\alpha \log^2 \varepsilon^{-1})$. ¿From numerics presented, we observe that the quantics tensor method has proved its value in application to various function related tensors/matrices arising in computational quantum chemistry and in the traditional FEM/BEM—the tool apparently works.

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1 Introduction

1.1 Evolution of tensor methods in the recent decade

In recent years, the idea of using the tensor-structured data formats was recognized as the basic concept for breaking down the "curse of dimensionality" in multidimensional numerical simulations. The guiding principle of tensor methods is an approximation of multivariate functions and operators relying on certain separation of variables. Modern applications include the high-dimensional problems arising in material sciences, bio-science, stochastic modeling, DMRG and quantum computations, signal processing, machine learning, financial mathematics.

The computational task is focused on the efficient low-complexity representation of higher order tensors and the related linear operators. In the current discussion, a tensor of order d, or briefly N-d tensor, is thought as the function on a product index set, $\mathbf{A} : I^{\otimes d} \to \mathbb{R}$ with d-fold product $I^{\otimes d} = I \times \cdots \times I$, and $I = \{1, ..., N\}$. The subsequent exponential scaling in the storage size, N^d,

predisposes the severe computational difficulties when using the traditional numerical algorithms that suffer from the "curse of dimension".

Recent approaches, like the wavelet multiscale methods [7, 8] and the hyperbolic cross (sparse grids) approximation [5, 41, 47] allow to relax the curse of dimension, and already make possible to treat the moderate dimensional problems, e.g., with $d \leq 10$.

Methods which allow the linear scaling in the dimension are distinctively linked with the idea of tensor approximation via separation of variables (see survey papers [33, 27] and references therein).

Application of the orthogonal rank-$(r_1, ..., r_d)$ Tucker tensor format (cf. [44, 9]) allows to relax the curse of dimension dramatically because of the reduced storage complexity, $O(r^d + drN)$, where, in practice, the sufficient maximal Tucker rank $r = \max\limits_{1\leq\ell\leq d} r_\ell$, can be much smaller than N, say, $r = O(\log N)$. The particular case of the Tucker representation, usually refereed as the canonical model, can be specified by the diagonal Tucker core with $r_\ell = r$, $(\ell = 1, ..., d)$ implying the linear storage scaling in d, drN. In general, the best r-term nonlinear approximation indicates the slow polynomial convergence in the rank parameter r, and it can be estimated by the simple greedy-type incremental algorithms [43]. For the class of (physically relevant) analytic multivariate functions and Green's kernels the exponential convergence in the separation rank r can be proved [14, 23, 25, 26], that leads to the asymptotically optimal bound on the canonical rank, $r = O(\log N)$.

Since the well-known limitations in approximation via canonical model [11], the mixed (two-level) orthogonal Tucker-canonical representation via imposing the rank-R canonical core tensor was introduced [23, 28]. It inherits the beneficial features of both models, orthogonality and linear scaling in d. The multigrid accelerated version of the mixed Tucker-canonical format was shown to be efficient in tensor computation of the 3D integral transforms in *ab initio* electronic structure calculations [28, 29].

The SVD-based approximation in the Tucker format was introduced, see the HOSVD approximation of the full format tensors [10], and RHOSVD approximation applied to the canonical targets [28]. These algorithms can be applied to moderate dimensions.

The rank-structured tensor formats that scale linear in the dimension d and, at the same time, allow the direct SVD-based truncated multilinear operations can be constructed using the idea of partial decoupling of dimensions. In computational molecular dynamics such methods are known for longer time as hierarchical or binary cascadic multi-configuration tensor methods (see [1, 34] for further details). Methods based on tensor product states representation (similar to TT/TC factorization below) became popular in density matrix renormalization group (DMRG) theory since [46], as well as in slightly entangled quantum computations [45]. The idea of dimension splitting in the context of the canonical tensor approximation was addressed in [23, Lemma 2.2].

The beneficial feature of the binary cascadic dimension splitting and DMRG methods is due to their linear scaling in d and N that can be realized by using the truncated SVD approximation or the truncated Schmidt decomposition (SD) that is another notation for truncated SVD, commonly used in physical literature. Recently, the tensor formats based on the tree-type or hierarchical dimension splitting have attracted much attention in mathematical community (see [37, 18, 4]). The non-hierarchical dimension splitting was introduced based on the so-called Three-dimensional Tensors [35], or equivalently Tensor Train (TT) [37] format. The storage is estimated by $O(dr^2N)$, where r is the maximal separation (splitting) rank. Furthermore, the quasi-optimal SVD-based algorithms for the rank optimization in hierarchical/TT dimension splitting schemes have been described in [37, 15].

In the present paper, we make use of the TT- and related formats in the framework of tensor-truncated function/operator calculus. In §2.1 below, the generalised *tensor chain* (TC) representation is addressed characterized by the periodic-type dimensional splitting scheme. It is motivated by the fact that from a physical point of view, periodic boundary conditions are normally highly

preferable to the open ones (the latter correspond to TT format) [46]. In §2.2, we discuss the two-level Tucker-TC model that is a combination of the orthogonal Tucker decomposition with the TT/TC-representation of the Tucker core. The advantage is that it provides linear storage scaling in the rank parameter due to the fact that both the maximal Tucker and TC ranks appear to be much smaller than N, $r \ll N$. The special case of above model is the two-level canonical-TT format that is proved to be useful in the tensor-structured operator calculus [30, 27].

1.2 Why folding of a tensor may lead to $\log N$-complexity

In high resolution molecular/electronic structure calculations, in FEM applications and in stochastic PDEs the univariate grid size N specifying N-d tensors resolving multiple singularities may be rather large, say, $N \approx 10^4$, that addresses the question on whether a better than linear asymptotic in N can be attained. The answer is yes, specifically, the asymptotic complexity $O(d \log N)$, i.e. logarithmic in the volume size, is possible if we deal with the "well structured" data. For example, it is known in signal processing, spectroscopy and higher-order statistics that the folding of a sampling vector into a matrix or 3-tensor may reduce the number of essential parameters (samplings) to reconstruct exactly the initial vector in $\mathbb{R}^N$ (cf. [42, 21, 39]). The relation to a separable representation of polyadics was emphasized in [20, 6].

To illustrate why the folding of a vector/tensor to a high-dimensional data format might lead to the compressed representation, we present the simple, but instructive example on the dyadic *folding of exponential vector*. The next statement is the particular case of the more general Lemma 2.5 below on the q-adic folding of N-vectors.

Proposition 1.1 *For a given $N = 2^L$, with $L \in \mathbb{N}_+$, and $c, z \in \mathbb{C}$, the single exponential vector $\mathbf{X} := \{x_n := cz^{n-1}\}_{n=1}^N \in \mathbb{C}^N$, can be reshaped by the successive dyadic folding to the rank-1 $\underbrace{2 \times 2 \times ... \times 2}_{L}$-tensor representation (shortly, to the rank-1, 2-L tensor),*

$$\mathbf{X} \mapsto \mathbf{A} = c \otimes_{p=1}^{L} \begin{bmatrix} 1 \\ z^{2^{p-1}} \end{bmatrix}, \quad \mathbf{A} : \{1,2\}^{\otimes L} \to \mathbb{C}. \tag{1.1}$$

The number of representation parameters is reduced dramatically from N to $2 + \log_2 N$.

Proposition 1.1 implies that the exponential N-vector is exactly represented by the rank-1, 2-L quantics tensor of size $2 \times 2 \times ... \times 2$ represented by only $2 + \log_2 N$ parameters. The similar folding strategy can be applied to matrices and N-d tensors (see §2.4). In the case of a general vector/matrix/tensor, the resultant 2-dL folding tensor can be *approximated* in the low rank TT/TC-format.

In the present paper, we make a step toward the almost grid-independent (or meshless) representation of high order tensors. We show that the quantics-TT (QTT) approximation of q-$\log_q N$ tensors obtained by the q-adic (or simply *quantics*[1] type) multidimensional folding, and applied to a class of function related N-vectors, $N \times N$-matrices or N-d tensors provides exponential convergence in the *canonical rank*. In particular, we prove that the "exponential, trigonometric and polynomial" vectors have fixed QTT-rank uniformly in the vector size N. This allows to understand why the multifolding of vectors/tensors may lead to the $d \log N$-computational complexity.

Notice that the terminology also mimics the representation via elementary information quantum ("quant") since the initial large vector is split into small fractions of size $q = 2, 3$ (*quantics*). This "pin-point" resolution allows to find the separable structure at all levels including the elementary

[1]The terminology is borrowed from the methods of separable representation of polyadics, see [6].

q-quants. Hence, the rank structured quantics approximation discovers the similarity patterns in the input data up to the finest resolution level, providing the way for the best possible compression rate within the chosen rank-structured dimensional splitting model posed in the auxiliary dimension $D = d \log_q N$.

We introduce the semianalytic constructive scheme providing the low rank quantics-TT approximation of function related tensors, that can be substantiated on the SVD-based rank reduction algorithm in [35].

1.3 Toward asymptotically optimal grid-based numerical methods

Tensor-structured numerical methods of the linear scaling $O(dN)$, are proved to be efficient for representation of functions and operators in the Hartree-Fock and Kohn-Sham models in electronic structure calculations [3, 28, 22]. Numerical method for solution of the Hartree-Fock equation by tensor truncated iteration was recently presented in [29]. Other successful applications to high-dimensional eigenvalue problems [19, 26] and to stochastic PDEs [32, 31] are reported. Using separation of variables in machine learning is addressed in [2]. Numerical examples in [36] demonstrated the highly compressed TT-approximation of $2^L \times 2^L$-matrices arising in FEM.

The QTT method developed in this paper has proved its value in tensor decomposition of large multi-dimensional data sets arising in traditional FEM, stochastic PDEs, and in numerical quantum chemistry—the tool apparently works. The particular numerical illustrations presented in Section 3.4 indicate surprisingly good compression rate $O(d \log N)$, of the QTT approximation applied to certain matrix-valued functions and function related tensors. This includes solutions of model boundary-value and eigenvalue problems in $\mathbb{R}^d$, as well as some examples of electron densities and Hartree potentials in electronic structure calculations. Moreover, DMRG calculations in [46, 45] show that QTC/QTT-type "matrix product states" tensor formats are indispensable in moder quantum computations.

1.4 Outline of the main results and future prospects

In the present paper we discuss the new prospects of tensor-structured data formats in high dimensional applications based on the idea of quantics representations.

The quantics-based tensor approximation methods are described applied to the discrete functions over the d-fold index set of size $N \times ... \times N$, or briefly N-d tensors, and to the related matrices representing the discrete analogues of differential-integral operators. For some classes of function related N-d tensors, we give the constructive proof on the $O(d \log N \log \varepsilon^{-1})$-complexity bound for their approximation up to the accuracy $\varepsilon > 0$, in the set of low rank q-D quantics tensors in auxiliary dimension $D = d \log_q N$, with small base $q = 2, 3$, such that $N = q^L$. In particular, we justify the low-rank quantics tensor approximation for solutions of certain elliptic boundary value/spectral problems in $\mathbb{R}^d$.

The quantics approximation of log-log scaling, $O(d \log N \log \varepsilon^{-1})$, opens the new perspectives for developing reliable computational methods in higher dimensions that are free from the "curse of dimensionality", noticeable limitations on the grid-size (kind of the meshless method), and from numerical instabilities. In the case of polynomially convergent FEM-FDM discretisations, i.e. for $\varepsilon = O(N^{-\alpha})$, $\alpha > 0$, we arrive at the QTT solution methods with the asymptotic complexity $O(d \log^{\beta} \varepsilon^{-1})$, $\beta \geq 2$, that seems to be the *nearly optimal computational cost* expected in the high dimensional numerical modeling.

With impetus to real life applications, we mention that the QTT method can be employed in the framework of truncated iteration or DMRG-type optimisation for solving classes of elliptic/parabolic equations in higher dimensions with log-scaling in the volume size.

The rest of the paper is organised as follows. Section 2 introduces the quantics (folding) tensor approximation. We prove that the exponential and trigonometric tensors allow the exact rank-1 (resp. rank-2) quantics representation, while the Chebyshev polynomial sampled over Chebyshev Gauss-Lobatto grid has separation rank 2 in quantics tensor format. Then we prove the approximation error estimate in terms of the canonical rank applied to the class of function related quantics tensors. Section 3.4 presents various numerical examples on the $O(D \log \varepsilon^{-1})$-approximation of N-d tensors by the D-dimensional q-D quantics with the auxiliary (vertual) dimension $D = d \log_q N$.

2 Approximation in quantics tensor formats

2.1 Basic rank-structured tensor representations

Tensors of order d are defined as the elements of finite dimensional tensor-product Hilbert space $\mathbb{W}_{\mathbf{n}} \equiv \mathbb{W}_{\mathbf{n},d}$ of the d-fold, $\underbrace{N_1 \times ... \times N_d}_{d}$ real/complex-valued arrays, and equipped with the Euclidean scalar product. Each tensor in $\mathbb{W}_{\mathbf{n}}$ can be represented componentwise, $\mathsf{A} = [A(i_1, ..., i_d)]$ with $i_\ell \in I_\ell := \{1, ..., N_\ell\}$, and $\mathbf{n} = (N_1, ..., N_d)$, where for the ease of presentation, we mainly consider the equal-size tensors, i.e., $I_\ell = I = \{1, ..., N\}$ $(\ell = 1, ..., d)$. We call the elements of $\mathbb{W}_{\mathbf{n}} = \mathbb{R}^{\mathcal{I}}$ with $\mathcal{I} = I_1 \times ... \times I_d$, as N-d tensors and use ceveral equivalent notations for the corresponding d-dimensional arrays, $\mathsf{A} \equiv \mathsf{A}_{(N,d)} \equiv \mathsf{A}_{(\mathbf{n},d)} \in \mathbb{W}_{\mathbf{n}}$. Dimension of the Hilbert space scales exponentially in d, $\dim \mathbb{W}_{\mathbf{n},d} = N^d$.

The rank-$(r_1, \ldots, r_d)$ *Tucker format* [44, 9]) contains all tensors in $\mathbb{W}_{\mathbf{n}} = \mathbb{R}^{\mathcal{I}}$, that can be presented in the form of a tensor-by-matrix *contracted product* over the product index set $J := \times_{\ell=1}^{d} J_\ell$, with $J_\ell = \{1, ..., r_\ell\}$, and $\mathbf{r} = (r_1, ..., r_d) \in \mathbb{N}_+^d$,

$$\mathsf{V} = \boldsymbol{\beta} \times_1 T^{(1)} \times_2 T^{(2)} ... \times_d T^{(d)} \in \mathbb{W}_{\mathbf{n}}, \tag{2.1}$$

and with certain (orthogonal) $N \times r_\ell$ side matrices, $T^{(\ell)} = [t_\ell^1 ... t_\ell^{r_\ell}] \in \mathbb{R}^{I \times J_\ell}$. The coefficients (core) tensor $\boldsymbol{\beta} = [\beta(\nu_1, ..., \nu_d)]$, $\nu_\ell \in J_\ell$, is an element of a (dual) tensor space $\mathbb{B}_{\mathbf{r}} = \mathbb{R}^{J_1 \times ... \times J_d}$. We denote this tensor class by $\boldsymbol{\mathcal{T}}_{\mathbf{r},\mathbf{n}} \subset \mathbb{W}_{\mathbf{n}}$. The storage size is still exponential, $O(r^d + drN)$, since, in general, the interdimensional connectivity tensor $\boldsymbol{\beta}$ is fully populated.

The rank-R *canonical format* is defined as the particular case of Tucker model (2.1) specified by equal ℓ-mode ranks, $r_\ell = R$ $(\ell = 1, ..., d)$, and by the diagonal Tucker core $\boldsymbol{\beta} := diag\{\beta_1, ..., \beta_R\}$, such that $\beta(\nu_1, ..., \nu_d) = 0$ except when $\nu_1 = ... = \nu_d$ with $\beta(\nu, ..., \nu) = \beta_\nu$. The orthogonality of $T^{(\ell)}$ is no longer required. We denote by $\boldsymbol{\mathcal{C}}_{R,\mathbf{n}}$ the class of tensors in $\mathbb{W}_{\mathbf{n}}$ whose rank does not exceed R, $rank(\mathsf{V}) \le R$. In spite of linear scaling in d, dRN, the inflexible and rather poor connectivity pattern of this format, parallel with the lack of orthogonality, lead to the well known computational difficulties with the canonical decomposition. Another possible drawback is the "rigid" constraints due to the equal rank distribution for all dimensions, $r_\ell = R$, $\ell = 1, ..., d$.

The rank-$\mathbf{r}$ *tensor train (TT) format* is defined in the spirit of Tucker model, but with essentially reduced "connectivity" constraints (see [35, 37]). As in the case of canonical format it scales linearly in both d and N. The generalisation of the TT-format to the case of "periodic" index chain is given by the following definition.

Definition 2.1 *(Tensor chain format). For the given rank parameter* $\mathbf{r} = (r_0, ..., r_d)$*, and the respective index sets* $J_\ell = \{1, ..., r_\ell\}$ $(\ell = 0, 1, ..., d)$*, with the periodicity constraints* $J_0 = J_d$ *(i.e.,* $r_0 = r_d$*), the rank-*$\mathbf{r}$ *tensor chain (TC) format contains all elements* V *in* $\mathbb{W}_{\mathbf{n}} = \mathbb{R}^{\mathcal{I}}$ *that can be represented as the chain of contracted products of 3-tensors over the d-fold product index set* $J := \times_{\ell=1}^{d} J_\ell$*,*

$$\mathsf{V} = \{\times_\ell\}_{\ell=1}^{d} \mathsf{G}^{(\ell)} \quad \textit{with 3-tensors} \quad \mathsf{G}^{(\ell)} \in \mathbb{R}^{J_{\ell-1} \times I_\ell \times J_\ell}, \tag{2.2}$$

or in the index notation,

$$V(i_1,...,i_d) = \sum_{\alpha_1 \in J_1} \cdots \sum_{\alpha_d \in J_d} G^{(1)}(\alpha_d, i_1, \alpha_1) G^{(2)}(\alpha_1, i_2, \alpha_2) \cdots G^{(d)}(\alpha_{d-1}, i_d, \alpha_d).$$

Denote this set of tensors by $TC[\mathbf{r}, d] \equiv TC[\mathbf{r}, \mathbf{n}, d] \subset \mathbb{W}_{\mathbf{n}}$ *(d can be skept upon the context).*

In the case $J_0 = J_d = \{1\}$ *(disconnected chain), this construction coincides with the respective definition of TT format in [35], thus implying* $TT[\mathbf{r}, d] \subset TC[\mathbf{r}, d]$.

The beneficial properties of the TC format are collected in the following lemma.

Lemma 2.2 *(A) Storage requirement for the rank-***r** *TC tensors in (2.2) is bounded by*

$$\sum_{\ell=1}^{d} r_{\ell-1} r_\ell \, N \le d r^2 N \quad \textit{with} \quad r = \max_\ell r_\ell.$$

(B) The rank-R canonical tensor belons to $TC[\mathbf{r}, d]$ *with* $\mathbf{r} = (R, ..., R)$. *TC rank of a tensor is the same in* $\mathbb{C}$ *and in* $\mathbb{R}$.
(C) Let $\mathbb{W} = \mathbb{W}_{\mathbf{n}}$ *be the tensor product of lower dimensional tensor product Hilbert spaces,*

$$\mathbb{W} := \bigotimes_{k=1}^{K} \mathbb{W}_k \quad \textit{with} \quad dim \mathbb{W}_k = d_k,$$

and let us suppose that the set of $TC[\mathbf{r}_k, d_k]$*-tensors in* $\mathbb{W}_k$ *is given by*

$$\mathbf{V}_k = \{\times_\ell\}_{\ell=1}^{d_k} \mathbf{G}_k^{(\ell)} \in TC[\mathbf{r}_k, d_k] \subset \mathbb{W}_k, \quad J^{(k)} := \times_{\ell=1}^{d_k} J_\ell^{(k)},$$

satisfying the compatibility conditions $J_{d_k}^{(k)} = J_{d_{k+1}}^{(k+1)}$ $(k = 1, ..., K-1)$. *Then the tensor product of* $\mathbf{V}_k$ $(k = 1, ..., K)$, *is a D-dimensional tensor with* $D = d_1 + ... + d_K$, *such that*

$$\mathbf{V} = \bigotimes_{k=1}^{K} \mathbf{V}_k \in TC[\mathbf{r}_D, D], \quad \textit{with} \quad \mathbf{r}_D = (\mathbf{r}_1, ..., \mathbf{r}_K), \quad \mathcal{J}_D = J^{(1)} \times ... \times J^{(K)}.$$

In the case $J_{d_k}^{(k)} = \{1\}$ $(k = 1, ..., K-1)$, *the product index set* $\mathcal{J}$ *represents the union of disjoint index chains.*

Proof. In the case $J_0 = J_d = \{1\}$, assertions (A) - (B) are proven in [35]. In the general case, items (A) - (B) can be verified by the similar arguments.

To prove (C), we concatenate $\mathbf{V}_k$ $(k = 1, ..., K)$, and check that the index set $\mathcal{J}_D = J^{(1)} \times ... \times J^{(K)}$ defines the d-fold index chain that satisfies Definition 2.1, with $D = d_1 + ... + d_K$, and $\mathbf{r}_D = (\mathbf{r}_1, ..., \mathbf{r}_K)$. In fact, this is true due to the compatibility conditions on the boarder indices in $J^{(k)}$, $J_{d_k}^{(k)} = J_{d_{k+1}}^{(k+1)}$, and the periodicity property $J_0^{(k)} = J_{d_k}^{(k)}$, imposed by Definition 2.1 applied to each $\mathbf{V}_k \in TC[\mathbf{r}_k, d_k]$ $(k = 1, ..., K)$. The last statement is straightforward. ∎

Applicability of the general TC format with $J_0 = J_d \neq \{1\}$, can be motivated, in particular, by the following computational tasks:

– DMRG computations of slightly entangled quantum systems [45, 46] with periodic boundary conditions.

– Approximation of symmetric/antisymmetric tensors.

– Rank optimization in the case of highly nonuniform distribution of the ℓ-mode, TT-rank parameters r_ℓ, $\ell = 1, ..., d$.

Notice that approximation of the full, canonical or TT-tensors by using the low TT-rank elements can be fulfilled by the noniterative procedure based on SVD/QR decompositions [35]. In the case of general TC tensors the rank reduction operations require certain modifications based on the use of simple ALS type iteration applied in the cyclic ordering similar to that for the familiar ALS iteration to compute the orthogonal Tucker approximation.

2.2 Combining Tucker, canonical, and TC formats

The rank-R two-level (mixed) Tucker-canonical format denoted by $\boldsymbol{\mathcal{T}}[\mathcal{C}_{R,\mathbf{r}}]$, contains all Tucker tensors in $\boldsymbol{\mathcal{T}}_{\mathbf{r},\mathbf{n}}$ with the Tucker core in $\boldsymbol{\mathcal{C}}_{R,\mathbf{r}}$ (see [23, 28]). This benefits from the linear storage complexity, $drN + dRr$, orthogonality, and the opportunity for *variable directional ranks*, $\mathbf{r} = (r_1, ..., r_d)$. Clearly, we have the imbedding $\boldsymbol{\mathcal{T}}[\mathcal{C}_{R,\mathbf{r}}] \subset \boldsymbol{\mathcal{C}}_{R,\mathbf{n}}$.

Similar to the previous construction, we introduce the *Tucker-TC format*, $\boldsymbol{\mathcal{T}}_{\mathbf{r}}[TC[\mathbf{r}_1]]$, containing all Tucker tensors in $\boldsymbol{\mathcal{T}}_{\mathbf{r},\mathbf{n}}$ with the Tucker core in the rank-$\mathbf{r}_1$ TC format. Now the storage complexity of representation scales linearly in r, $O(drN + d\, r_1^2\, r)$, while the representation basis is given explicitly by the "optimal" set of orthogonal Tucker vectors. This may be gainfully applied in the framework of the Galerkin scheme. Notice that the rank-R, $\boldsymbol{\mathcal{T}}[\mathcal{C}_{R,\mathbf{r}}]$-format is embedded into the class $\boldsymbol{\mathcal{T}}_{\mathbf{r}}[TT[\mathbf{r}_1]]$ with $\mathbf{r}_1 = (R, ..., R)$ (cf. Lemma 2.2, (B)). Hence, the further TT-rank optimisation of the initial element in $\boldsymbol{\mathcal{T}}_{\mathbf{r}}[TT[\mathbf{r}_1]]$, can be accomplished with the SVD-based scheme applied to the small size canonical core tensor in $\boldsymbol{\mathcal{C}}_{r_1,\mathbf{r}}$, $(r \ll N)$.

Another tensor format that might be useful in numerical multilinear algebra is specified as a set of N-d tensors in $\boldsymbol{\mathcal{C}}_{R,\mathbf{n}}$ with $N = q^L$, where each canonical N-vector in rank-1 terms is represented by the q-L tensor in the $TC[\mathbf{r}, L]$ format with $L = \log_q N$. We denote this *canonical-TC format* by $\boldsymbol{\mathcal{C}}_{R,\mathbf{n}}[TC[\mathbf{r}, L]]$. The particular representation looks like

$$\mathbf{V} = \sum_{k=1}^{R} c_k T_k^{(1)} \times_2 T_k^{(2)} ... \times_d T_k^{(d)} \in \boldsymbol{\mathcal{C}}_{R,\mathbf{n}}[TC[\mathbf{r}, L]], \tag{2.3}$$

where, for $k = 1, ..., R, \nu = 1, ..., d$,

$$T_k^{(\nu)} := \{\times_\ell\}_{\ell=1}^{L} \mathbf{G}_{k,\nu}^{(\ell)} \in TC[\mathbf{r}, L] \quad \text{with small-size 3-tensors} \quad \mathbf{G}_{k,\nu}^{(\ell)} \in \mathbb{R}^{r_{\ell-1} \times q \times r_\ell}.$$

The storage complexity of respective representation scales logarithmically in N, $O(Rr^2 d \log N)$, hence, it has advantages for large tensor size N.

Based on Lemma 2.2,(D), the tensors in $\boldsymbol{\mathcal{C}}_{R,\mathbf{n}}[TC[\mathbf{r}, \mathbf{q}, L]]$ can be presented as the R-term sum of elements in $TC[\mathbf{r}_D, D]$, leaving in the higher dimensional space with $D = dL$, and with the d-fold multiindex index $\mathbf{r}_D = (\mathbf{r}, ..., \mathbf{r})$.

2.3 Low rank quantics representation of vectors

In this Section, we prove the basic result saying that the class of discrete exponential (resp. trigonometric) N-vectors allows the rank-1 (resp. rank-2) q-folding representation with small $q = 2, 3, ...$, that reduces the storage complexity from linear $O(N)$ to the logarithmic one $O(q \log_q N)$.

Given $q = 2, 3, ...$, we suppose that $N = q^L$ with some $L = 1, 2, ...$ The folding (lifting) and unfolding (reducing) transforms on N-d tensors can be interpreted as the dual reshaping operations specified by the reordering scheme of the respective index sets. Next definition introduces the folding of N-d tensors into the elements of auxiliary D-dimensional tensor space with $D = d \log_q N$.

Definition 2.3 *Introduce the q-adic folding transform of degree $2 \le p \le L$,*

$$\mathcal{F}_{q,d,p} : \mathbb{W}_{\mathbf{n},d} \to \mathbb{W}_{\mathbf{m},dp}, \quad \mathbf{m} = (\mathbf{m}_1, ..., \mathbf{m}_\ell), \quad \mathbf{m}_\ell = (m_{\ell,1}, ..., m_{\ell,p}),$$

with $m_{\ell,1} = q^{L-p+1}$, and $m_{\ell,\nu} = q$ for $\nu = 2, ..., p$, $(\ell = 1, ..., d)$, that reshapes the initial $\mathbf{n}$-d tensor in $\mathbb{W}_{\mathbf{n},d}$ to the quantics space $\mathbb{W}_{\mathbf{m},dp}$ as follows:
(A) For $d = 1$ a vector $\mathbf{X}_{(N,1)} = [X(i)]_{i \in I} \in \mathbb{W}_{N,1}$, is reshaped to the element of $\mathbb{W}_{q^{L-p+1},p}$ by

$$\mathcal{F}_{q,1,p} : \mathbf{X}_{(N,1)} \to \mathbf{Y}_{(\mathbf{m},p)} = [Y(\mathbf{j})] := [X(i)], \quad \mathbf{j} = \{j_1, ..., j_p\},$$

with $j_1 \in \{1,...,q^{L-p+1}\}$, *and* $j_\nu \in \{1,...,q\}$ *for* $\nu = 2,...,p$. *For fixed* i, $j_\nu = j_\nu(i)$ *is defined by* $j_\nu = 1 + C_{L-p-1+\nu}$, $(\nu = 1,...,p)$, *where the* $C_{L-p-1+\nu}$ *are found from the partial radix-q representation of* $i-1$,

$$i - 1 = C_{L-p} + C_{L-p+1}q^{L-p+1} + \cdots + C_{L-1}q^{L-1}.$$

(B) For $d > 1$ *a tensor* $\mathbf{A}_{(\mathbf{n},d)} = [A(i_1,...,i_d)]$, $\quad i_\ell \in I_\ell$, $\ell = 1,...,d$, *is reshaped by*

$$\mathcal{F}_{q,d,p} : \mathbf{A}_{(\mathbf{n},d)} \to \mathbf{B}_{(\mathbf{m},dp)} = [B(\mathbf{j}_1,...,\mathbf{j}_d)] := [A(i_1,...,i_d)], \quad \mathbf{j}_\ell = \{j_{\ell,1},...,j_{\ell,p}\},$$

with $j_{\ell,1} \in \{1,...,q^{L-p+1}\}$, *and* $j_{\ell,\nu} \in \{1,...,q\}$, *for* $\nu = 2,...,p$, *and for all* $\ell = 1,...,d$. *Now the univariate* ℓ*-mode index* i_ℓ *is reshaped into* $\mathbf{j}_\ell$ *as in the case* $d = 1$. *For completeness, in the case* $p = 1$, *we define* $\mathcal{F}_{q,d,1}$ *as the identity mapping.*

(C) For the maximal degree folding ($p = L$), *the multiindex* $\mathbf{j}_\ell - \mathbf{1}$ *with* $j_{\ell,\nu} \in \{1,...,q\}$, *is the q-adic representation of* $i_\ell - 1$, $i_\ell \in I_\ell$, *in radix-q system, i.e.,*

$$j_{\ell,\nu} = 1 + C_\nu, \quad \nu = 1,...,L, \quad \textit{where} \quad i_\ell - 1 = \sum_{\nu=1}^{L} C_\nu q^{\nu-1}.$$

Definition 2.4 *The set of tensors in* $\mathbb{W}_{\mathbf{m},dL}$, *which can be represented in* $TT[\mathbf{r}]$ *(resp.* $TC[\mathbf{r}]$*) format will be called as* $QTT[\mathbf{r}]$ *(resp.* $QTC[\mathbf{r}]$*) tensors.*

Example 1. Quantics folding of the exponential N-vector: $\mathbf{X} = [1\, z\, z^2\, z^3\, z^4\, z^5\, z^6\, z^7]^T \in \mathbb{C}^8$, with $N = 2^3$, $L = 3$, $\mathcal{F}_{2,3}(\mathbf{X}) \in \mathbb{C}^{2\times 2\times 2}$,

$$\mathcal{F}_{2,3} : \mathbf{X} \mapsto \mathbf{A} = \begin{bmatrix} 1 \\ z \end{bmatrix} \otimes \begin{bmatrix} 1 \\ z^2 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ z^4 \end{bmatrix} \in QTT[\mathbf{1}].$$

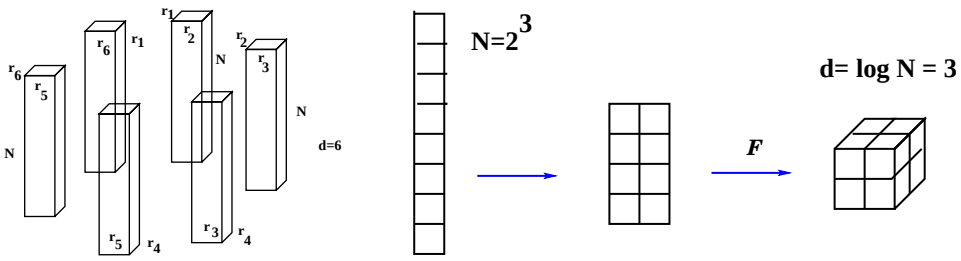

Figure 2.1: TC-model for $d = 6$ (left); Quantics folding of a vector, $L = 3$ (right).

Example 2. For $d = 1$ and $p = 2, 3$, the reshaping map $\mathcal{F}_{q,1,p}$ folds an N-vector to a $N/q \times q$-matrix or to $N/q^2 \times q \times q$, 3-tensor, respectively.

For the sake of higher compressibility, the *maximal degree folding*, $\mathcal{F}_{q,d,L}$, has to be used.

The unfolding transform, e.g., tensor-to-matrix (matricization) or tensor-to-vector (vectorization), may be viewed as the reverse to the folding, $\mathcal{F}^{-1}_{q,d,p}$, and it can be also defined in the conventional way [33].

The folding transform $\mathcal{F}_{q,d,p}$ exhibits the following useful properties:

(F1) $\mathcal{F}_{q,d,p}$ is the linear isometry between $\mathbb{W}_{N,d}$ and $\mathbb{W}_{q^{L-p+1},dp}$ that has the inverse transform (unfolding) $\mathcal{F}^{-1}_{q,d,p} : \mathbb{W}_{q^{L-p+1},dp} \to \mathbb{W}_{N,d}$.

(F2) The q-folding of a rank-1 tensor $w = x_1 \times ... \times x_d \in \mathbb{W}_{N,d}$, is given by the outer product of componentwise reshaping transforms of canonical vectors,

$$\mathcal{F}_{q,d,p} w = \mathcal{F}_{q,1,p} x_1 \otimes ... \otimes \mathcal{F}_{q,1,p} x_d.$$

(F3) Let $d = 1$, then for any $p = 2, ..., L$ and $\mathbf{X} = [X(i)] \in \mathbb{C}^N$, we have the following bound on the TT rank of the quantics image $\mathcal{F}_{q,1,L}\mathbf{X}$,

$$r_{p-1} \leq rank(\mathbf{X}_p),$$

where $\mathbf{X}_p$ is the reshaping of $\mathbf{X}$ to a $N/q^{p-1} \times q^{p-1}$ matrix.

Next two lemmas present the basic results on the rank-1 (resp. rank-2) q-folding representation of the exponential (resp. trigonometric) vectors.

Lemma 2.5 *For given $N = q^L$, with $q = 2, 3, ...$ and $L \in \mathbb{N}_+$, and for given $c_k, z_k \in \mathbb{C}, \alpha_k \in \mathbb{R}$ $(k = 1, ..., R)$, we have (A) a sum of exponential N-vectors, $\mathbf{X} := \{x_n := \sum_{k=1}^{R} c_k z_k^{n-1}\}_{n=1}^{N}$, can be reshaped by the q-folding $\mathcal{F}_{q,1,L}$, to the rank-R, q-L tensor in $\mathbb{W}_{\mathbf{q},L}$,*

$$\mathcal{F}_{q,1,L} : \mathbf{X} \to \mathbf{A}_{(q,L)} = \sum_{k=1}^{R} c_k \otimes_{p=1}^{L} [1\ z_k^{q^{p-1}} \ ... \ z_k^{(q-1)q^{p-1}}]^T \in \boldsymbol{\mathcal{C}}_{R,\mathbf{q}}[TT[\mathbf{1}]]. \tag{2.4}$$

(B) A sum of trigonometric N-vectors, $\mathbf{X} := \{x_n := \sum_{k=1}^{R} c_k \sin(\alpha_k(n-1))\}_{n=1}^{N}$, can be reshaped to the rank-$2R$, q-L tensor $\mathbf{A}_{(q,L)}$, whose TT-rank do not exeed $2R$,

$$\mathcal{F}_{q,1,L} : \mathbf{X} \to \mathbf{A}_{(q,L)} = \sum_{k=1}^{R} \mathbf{A}_k \in \mathbb{W}_{q,L}, \quad with \quad \mathbf{A}_k \in TT[\mathbf{2}, L].$$

In both cases, the number of representation parameters is reduced from $(N+1)R$ to $(qL+1)R$ and $4qLR$, respectively.

Proof. (A) First, we consider the case of single exponential, $R = 1$. The proof follows by induction. For $L = 2$, i.e., $N = q^2$, the rank-1 representation can be directly verified by applying the vector-to-matrix folding,

$$\mathcal{F}_{q,1,2} : \mathbf{X}_{(q^2,1)} \to \mathbf{A}_{(q,2)} := \begin{pmatrix} 1 & z^q & \dots & z^{(q-1)q} \\ z & \ddots & \dots & z^{(q-1)q+1} \\ \vdots & \vdots & \ddots & \vdots \\ z^{q-1} & z^{2q-1} & \dots & z^{q^2-1} \end{pmatrix} = \begin{bmatrix} 1 \\ z \\ \vdots \\ z^{q-1} \end{bmatrix} [1\ z^q \ ... \ z^{(q-1)q}].$$

To prove the induction step from L to $L+1$, i.e., for $N = q\,q^L$, we define the subvectors $x_1, ..., x_q \in \mathbb{R}^{q^L}$ of $\mathbf{X}_{(N,1)}$ by $x_k(i) := \mathbf{X}[i + (k-1)q^L, 1]$, $(k = 1, ..., q,\ i = 1, ..., q^L)$, and then represent the result of a folding transform with $p = 2$, by the rank-1, $N/q \times q$-matrix via rescaling of the first subvector x_1,

$$\mathcal{F}_{q,1,2} : \mathbf{X}_{(N,1)} \to \mathbf{A}_{(N/q,2)} := c[x_1 x_2 ... x_q] = c x_1 \otimes y,$$

where the vector of scaling coefficients is given by $y := [1\ z^{q^L}\ ...\ z^{(q-1)q^L}]^T$. Now substitution of each matrix column x_k, $k = 1, ..., q$, of size $N/q = q^L$ by rank-1 tensor as in (2.4) leads to

$$\mathbf{A}_{(q,L+1)} = \left[\otimes_{p=1}^{L}[1\ z^{q^{p-1}}\ ...\ z^{(q-1)q^{p-1}}]^T\right] \otimes [1\ z^{q^L}\ ...\ z^{(q-1)q^L}]^T,$$

completing the induction step.

(B) Again, we begin from the case $R = 1$. Using trigonometric identity $\sin z = \frac{e^{iz}-e^{-iz}}{2i}$, and applying item (A) with $R = 1$, we arrive at the required claim on tensor rank of $\mathbf{A}_{(q,L)}$ over field $\mathbb{C}$. Now, the rank of each ℓ-mode unfolding matrix of the q-L tensor does not exceed 2, since the matrix rank does not change if we extend the field $\mathbb{R}$ to $\mathbb{C}$ (cf. Lemma 2.2, (B)). Since the TT-ranks do not exceed the ranks of respective directional unfolding matrices (cf. [37]), the maximal TT-rank of the q-L tensor $\mathbf{A}_{(q,L)}$ is bounded by $2R$.

In the case of arbitrary rank parameter $R > 1$, the result is obtained by summation of rank-1 (resp. rank-2) terms. The complexity bounds then follow from Lemma 2.2,(A). ∎

It turns out that the exponential-trigonometric product vector allows the $4\log_q N$ complexity quantics representation as proven by the following lemma.

Lemma 2.6 *For given $N = q^L$, with $q = 2, 3, ...$, $L \in \mathbb{N}_+$, and $c, z \in \mathbb{C}, \alpha \in \mathbb{R}$, the exponential-trigonometric vector $\mathbf{X} := \{x_n := cz^{n-1}\sin(\alpha(n-1))\}_{n=1}^N$, can be reshaped to a q-L tensor, $\mathcal{F}_{q,1,L} : \mathbf{X} \to \mathbf{A}_{(q,L)} \in TT[2]$, whose both canonical and TT-ranks do not exceed 2.*

Proof. The properties of the folding transform $\mathcal{F}_{q,1,L}$ imply that the q-L tensor $\mathbf{A}_{(q,L)}$ is obtained by the Hadamard product of the rank-1 quantics representation for a single exponential and rank-2 quantics of the trigonometric vector (cf. Lemma 2.5). Now, the statement follows from the fact that the Hadamard product with rank-1 tensor does not enlarge the TT-rank of the second factor that is exactly 2. Hence, the TT-rank of the resultant q-L tensor $\mathbf{A}_{(q,L)}$ does not exceed 2. ∎

Clearly, a R-term sum of exponential-trigonometric vectors with $N = q^L$, can be reshaped to the q-L tensor of complexity $O(Rq\log_q N)$ that follows by combining Lemma 2.5, and 2.6.

Remark 2.7 *The minimization of the parametric function $f_x(q) := q\log_q x$ for the large value of $x \in \mathbb{R}_+$, leads to the optimal folding base $q^* \in [2, 3]$. This means that for large vector-size N, the choice $q = 2, 3$ leads to the best compression rate. In the case $q = 2$, we have binary coding representation for the quantics index $\mathbf{j}(i) \in \{1, 2\}^{\otimes L}$, $i = 1, ..., N$ (cf. Def. 2.3, (C)).*

Next statement characterises the QTT rank bound for "polynomial" vectors.

Proposition 2.8 *Property (F3) of the quantics folding ensures that the QTT rank of the quantics image of any N-vector obtained by the equidistant sampling of a polynomial does not exceed $m+1$, where m is the polynomial degree. In fact, the column space of the reshaped matrix is spaned by at most $m+1$ polynomial vectors generated by monomials $1, x, ..., x^m$.*

Simple extension to the case of piecewise polynomial N-vectors is straightforward. In particular, quantics format applies to piecewise polynomial *wavelet basis functions*. For example, we can easily prove that the QTT rank of Haar wavelet does not exceed 2, implying that the asymptotic QTT compression properties are at least as good as for the Haar wavelets. "Mexican hat" wavelets generated by Gaussian-times-polynomials can be shown to have low QTT rank as well (see Remark 2.10).

Notice that the rank bound for hierarchical-Tucker tensors applied to the quantics image of a polynomial vector on equidistant grids is shown to be bounded by $O(m)$, where m is the polynomial degree, see [16].

It is worth to mention that using *equidistant sampling points is non mandatory.* In some cases the separation rank in the quantics tensorization may be reduced by using special grading of sampling points. In the next statements, we give some results on the rank bound in the case of polynomial vectors at $N+1$ Chebyshev Gauss-Lobatto nodes $x_j = \cos\frac{\pi j}{N} \in [-1,1],\ j = 0,...,N$, and for Gaussian type function with quadratic mesh grading.

Lemma 2.9 *(A) For any $n = 0,1,...$, the Chebyshev polynomial $T_n(x)$, $|x| \le 1$, sampled over $N+1$ Chebyshev nodes $x_j \in [-1,1]$, can be represented in the quantics space of 2-log N tensors with both $\mathbb{C}$-rank and QTT-rank ≤ 2, uniformly in N.*
(B) Any polynomial of degree m sampled over $N+1 = 2^L$ Chebyshev nodes at $[-1,1]$ has a quantics-TC separation rank bounded by $2m+1$.

Proof. (A) First we note that the Chebyshev polynomial $T_n(x) = \cos(n \arccos x)$, sampled at Chebyshev nodes coinsides with the cos-trigonometric vector sampled over uniformly graded points in variable $\theta_j = \arccos x_j$, $j = 0,...,N$. Then the result follows by Lemma 2.5.

(B) Any polynomial of degree m can be represented in the orthogonal basis of Chebyshev polynomials by at most $m+1$ terms with $T_0 = 1$. Hence (B) follows from item (A). ∎

Lemma 2.9 may be applied to the case of polynomial interpolation over Chebyshev nodes, which are usually more prefarable compared with equispaced nodes. In fact, this prevents the well-known instability appearing in those interpolation process based on equidistant grids.

Remark 2.10 *The TT-rank of the q-folded discrete Gaussian type function sampled over the uniform grid, $\{e^{-\alpha(n-1)^2}\}_{n=1}^N$, appears to be greater than 2, but numerical tests show that it remains to be almost uniformly bounded in the vector size N (see Table 3.1 below). Lemma 2.5 implies the rank-1 quantics representation in the case of quadratic mesh grading toward the origin, i.e., by sampling the Gaussian $e^{-\alpha t^2}$ over $t_n = \sqrt{h(n-1)}$, $(n = 1,...,N,\ h > 0)$.*

Conjecture 2.11 *Based on our extensive numerical tests, we further assume that the Gaussian-, polynomial- and sinc-vectors obtained via the uniform sampling, allow the quantics approximation by the q-folding, whose TT-rank remains bounded by a small constant (say, 4) uniformly in the vector size N (see Table 3.1).*

To complete this section, we notice that the previous results can be applied to R-term sums of exponential/trigonometric vectors in d dimensions, i.e., to the respective N-d tensors,

$$\mathbf{A}_{(\mathbf{n},d)} := \{x_{\mathbf{n}} := \sum_{k=1}^{R} c_k \prod_{\ell=1}^{d} z_{k,\ell}^{n_\ell - 1}\}_{\mathbf{n}\in I^{\otimes d}}, \quad I = \{1,...,N\}, \tag{2.5}$$

$$\mathbf{A}_{(\mathbf{n},d)} := \{x_{\mathbf{n}} := \sum_{k=1}^{R} c_k \prod_{\ell=1}^{d} \sin(\alpha_{k,\ell}(n_\ell - 1))\}_{\mathbf{n}\in I^{\otimes d}}, \quad I = \{1,...,N\}. \tag{2.6}$$

These tensors can be reshaped to the quantics formats $\boldsymbol{\mathcal{C}}_{R,\mathbf{q}}[TT[\mathbf{1}, dL]]$ (complexity $dqR\log_q N$) and $\boldsymbol{\mathcal{C}}_{R,\mathbf{q}}[TT[\mathbf{2}, dL]]$ (complexity $4dqR\log_q N$), respectively.

2.4 Analytic quantics approximation of function related tensors

In the following, we generalize the quantics representation of exponential-trigonometric N-vectors to the case of more general class of multidimensional N-d tensors. To describe the analytic tensor approximation, let us consider the class of function related tensors generated by certain analytic

functions f that allow the efficient approximation in the set of exponential sums on $[a,b] \subset \mathbb{R}_+$. In particular, such approximations can be based on the sinc method.

Now we prove the error bound for the *semianalytic quantics approximation* of function related tensors.

Lemma 2.12 *Suppose that for given continuous function $f : [a,b] \to \mathbb{R}$, and given $\varepsilon > 0$, there is an approximation by exponential sum, such that*

$$\max_{x\in[a,b]} |f(x) - \sum_{k=1}^{M} c_k e^{-t_k x}| \le \varepsilon. \tag{2.7}$$

Then for any $N = q^L$, with some $q = 2, 3, ...$, and $L \in \mathbb{N}_+$, we have:

(A) The function related N-d tensor $\mathsf{F} = [F_{\mathbf{i}}]$, defined by the entries

$$F_{\mathbf{i}} = f(hi_1 + hi_2 + ... + hi_d), \quad \mathbf{i} \in I^{\otimes d}, \quad h > 0, \quad \text{where } a \le dh \le b/N,$$

and discretising the multivariate function $g = f(\sum_{\ell=1}^{d} x_\ell)$ over the uniform grid imbedded into the region $a \le \sum_{\ell=1}^{d} x_\ell \le b$, can be represented by the rank-M, q-dL tensor up to the tolerance ε in the max-norm.

(B) Under the condition $a \le dh \le b/N$, the function related N-d tensor $\mathsf{G} = [G_{\mathbf{i}}]$, with the entries

$$G_{\mathbf{i}} = f(\sum_{\ell=1}^{d} x^2_{\ell,i_\ell}), \quad x_{\ell,i_\ell} = \sqrt{hi_\ell}, \quad \mathbf{i} \in I^{\otimes d},$$

discretising the multivariate function $g = f(\sum_{\ell=1}^{d} x_\ell^2)$ on the polynomially graded grid $\{x_{\ell,i_\ell}\}$, imbedded into the region $a \le \sum_{\ell=1}^{d} x_\ell^2 \le b$, can be represented by the rank-M, q-dL tensor with the tolerance ε in the max-norm.

In both cases, the number of representation parameters is bounded by $O(dqM \log_q N)$.

(C) Let Conjuncture 2.11 be valid, the approximation properties by Gaussian sums via the uniform sampling, i.e., for $x_{\ell,i_\ell} = hi_\ell$, ($\ell = 1, ..., d$), remain essentially the same except that the rank-M, q-dL tensor should be substituted by M-term sum of low-rank TT approximands representing each individual Gaussian vector.

Proof. Items (A), (B) directly follow from (2.5) and (2.6). Item (C) is justified by combining (2.5), (2.6), Remark 2.10 and Conjuncture 2.11 related to representation by Gaussian sums. ∎

Lemma 2.12 allows us to derive the accurate $O(d \log N)$-approximations to the wide class of function related tensors in high dimension. For a class of analytic functions the basic approximability assumption (2.7) can be verified with

$$\varepsilon = O(e^{-\alpha M/\log M}), \quad \alpha > 0,$$

by applying the *sinc*-approximation [17, 23, 25]. Notice that the semianalytic quantics approximations via Lemma 2.12 can be further optimised by applying the rank-r, $r < M$, TC approximation.

Quantics representations similar to those in Lemma 2.12 can be derived based on the product-polynomial or product-trigonometric, exponentially convergent approximations, analogues to (2.7). To this end, see also Conjuncture 2.11.

3 $O(d \log N)$-solution of elliptic/parabolic problems

In this section, we show how the QTT approximation method can be applied in the framework of truncated iteration for solving certain elliptic/parabolic equations in higher dimensions, providing log-scaling in the volume size N^d. Numerical illustrations are provided.

We shall frequently use the finite difference negative d-Laplacian, that allows the Kronecker rank-d representation,

$$\Delta_d = A \otimes I_N \otimes ... \otimes I_N + I_N \otimes A \otimes I_N ... \otimes I_N + ... + I_N \otimes I_N ... \otimes A \in \mathbb{R}^{I^{\otimes d} \times I^{\otimes d}}, \tag{3.1}$$

with $A = \Delta_1 = \text{tridiag}\{1, -2, 1\} \in \mathbb{R}^{N \times N}$, and I_N being the $N \times N$ identity.

Notice that the TT-rank of Δ_d is equal to 2 for any dimension (cf. [37]), while its QTT rank can be shown to be bounded by 4.

3.1 Representing model equations in low rank QTT format

Examples below demonstrate that some classes of boundary-value/eigenvalue problems may have solutions that are well approximated in the quantics formats.

Example 3. In the case of Schrödinger equation for hydrogen atom,

$$(-\frac{1}{2}\Delta - \frac{1}{\|x\|})u = \lambda u, \quad x \in \mathbb{R}^3, \quad u \in H^1(\mathbb{R}^3),$$

the physically relevant eigenpair with minimal eigenvalue is given by $u_1(x) = e^{-\|x\|}$, $\lambda_1 = -0.5$, hence both the solution $e^{-\|x\|}$, and the potential $\frac{1}{\|x\|}$, can be proven to provide accurate approximation in the low rank binary folding format, due to Lemma 2.12, and applying the *sinc*-quadrature approximation in [23, 25] (see Tables 3.2 and 3.3 for numerical illustrations).

Example 4. The eigenvectors $U_{\mathbf{i}}$, $\mathbf{i} \in I^{\otimes d}$, of the algebraic eigenvalue problem

$$\Delta_d U = \lambda U, \quad U \in \mathbb{R}^{N^d \times N^d},$$

are exactly in the rank-2 quantics tensor format with the oscillating trigonometric canonical vectors, $U_{\mathbf{i}} = \bigotimes_{\ell=1}^{d} \sin(i_\ell x_\ell)$. Representation (2.6) allows us to verify that this tensor is in the rank-2, q-quantics format for any $q = 2, 3, ...$

Example 5. The solution of the discrete Poisson equation in $\mathbb{R}^d$,

$$\Delta_d U = F \quad \text{with rank-1 r.h.s.} \quad F = \otimes_{\ell=1}^{d} f_\ell, \quad f_\ell \in \mathbb{R}^N, \tag{3.2}$$

is (approximately) represented in the rank-$(2M+1)$, tensor format,

$$U = \Delta_d^{-1} F \simeq U_M := \sum_{k=-M}^{M} c_k \bigotimes_{\ell=1}^{d} \exp(-t_k \Delta_1)\, f_\ell, \tag{3.3}$$

$$t_k = e^{k\mathfrak{h}}, \quad c_k = \mathfrak{h} t_k, \quad \mathfrak{h} = \pi/\sqrt{M}, \quad \Delta_1 \in \mathbb{R}^{N \times N},$$

providing the exponential convergence rate in the rank parameter, [14],

$$\left\| \Delta_d^{-1} F - U_M \right\| \le C e^{-\pi\sqrt{M}} \|F\|.$$

Hence, the low-rank approximability of the univariate vectors f_ℓ in the QTT format implies the desired property for the solution U_M.

3.2 Quantics representation of matrices on N-d tensors

Matrices acting on TC[**r**,d] tensors can be determined by their componentwise matrix-vector products with the univariate representation vectors of the test rank-1 tensors.

Definition 3.1 *We say that a matrix $\mathcal{A}$ acting on TC[**r**,$\mathcal{I}$,d] tensors belongs to the class of Kronecker rank-**m** matrices, TC[**m**,$\mathcal{K}\times\mathcal{I}$,d], if for each rank-1 element $\mathbf{V}\in$TC[**1**,$\mathcal{I}$,d], the resultant matrix-vector product is a d-tensor on the index set $\mathcal{K}$, $\mathcal{A}\mathbf{V}\in$ TC[**m**,$\mathcal{K}$,d], where $\mathbf{m}=(M_0,...,M_d)$, $M_0=M_d$. Using the Kronecker product notation,*

$$\mathcal{A}=\bigotimes_{\ell=1}^{d}\mathcal{A}^{(\ell)},\quad \mathcal{A}^{(\ell)}:\mathbb{R}^{I_\ell}\to\mathbb{R}^{M_{\ell-1}\times K_\ell\times M_\ell},$$

the explicit representation in the case of rank-1 input vector $\mathbf{V}=v_1\times...\times v_d$, is given by

$$\mathcal{A}\mathbf{V}=\bigotimes_{\ell=1}^{d}\mathcal{A}^{(\ell)}v_\ell,\quad \textit{where}\quad \mathcal{A}^{(\ell)}v_\ell\in\mathbb{R}^{M_{\ell-1}\times K_\ell\times M_\ell}.$$

*The action of $\mathcal{A}$ on the general tensor in TC[**r**,$\mathcal{I}$,d] is defined as an element of the TC[**p**,$\mathcal{K}$,d] format specified by the componentwise product $P:=J\odot M$ of index sets $J=J(\mathbf{r})$ and $M=M(\mathbf{m})$, with the respective Hadamard-product rank parameter, $\mathbf{p}=\mathbf{m}\odot\mathbf{r}$.*

Next lemma shows that the diagonal matrices generated by the exponential and trigonometric vectors can be proven to have fixed quantics Kronecker rank.

Lemma 3.2 *Quantics Kronecker-TT rank of the diagonal matrices generated by the exponential and trigonometric vectors of size $N=q^L$, equals 1 and 2, respectively.*

Proof. Notice that the matrix-vector product with the diagonal matrix is represented as the Hadamard product with the diagonal vector, then using Definition 3.1, the result follows from the respective bounds on the QTT-rank of the folded exponential/trigonometric vectors. ∎

The analysis of the low QTT-rank approximations of elliptic operator inverse is based on certain assumptions on the QTT-rank of the matrix exponential family for $d=1$.

Conjecture 3.3 *For any given $\varepsilon>0$, and for fixed $a,b>0$, let us assume that the family of matrix exponentials, $\{\exp(-t_k\Delta_1)\}$, $t_k>0$, $k=-M,...,M$, allows the rank-r_Δ, QTT ε-approximation, with r being uniformly bounded in the grid size N and scaling factors $t_k\in[a,b]\subset\mathbb{R}_{>0}$ (see Table 3.4 for numerical justification).*

With the previous assumption on the QTT-rank of the family of "univariate" matrix exponentials, $\{\exp(-t_k\Delta_1)\}$, $t_k>0$, we prove the following Lemma.

Lemma 3.4 *Under conditions of Conjecture 3.3 the representation (3.3) approximates the exact solution U up to the relative tolerance $\varepsilon>0$, and it has the complexity $O(dr_\Delta\log^2\varepsilon\log N)$, that scales logarithmically in both N and ε. Moreover, the matrix*

$$\mathcal{B}_M:=\sum_{k=-M}^{M}c_k\bigotimes_{\ell=1}^{d}\exp(-t_ka_\ell\Delta_1),\quad a_\ell>0,\quad \ell=1,...,d, \tag{3.4}$$

possesses the rank-$O(\log^2\varepsilon)$, QTT quantics ε-approximation (or preconditioner if M is small) to the anisotropic d-Laplacian inverse $\Delta_{d,\alpha}^{-1}$, where

$$\Delta_{d,\alpha}:=\sum_{\ell=1}^{d}a_\ell\bigotimes_{k=1}^{d}\Delta_1^{\delta_{\ell,k}},\quad \delta_{\ell,k}\quad \textit{is the Kronecker symbol.} \tag{3.5}$$

3.3 QTT-truncated iteration for elliptic/parabolic equations

QTT format can be utilized in the concept of approximate (truncated) iterations based on use of the rank structured formats to represent matrix-vector operations in the framework of *preconditioned iterative solvers* (cf. [25, 19, 26]). In our applications, we choose the manifold $\mathcal{S} = \mathcal{S}_{\mathbf{r}}$ of rank-$\mathbf{r}$, QTT tensors, and then perform the truncated iteration over this nonlinear manifold by "projection" the current iterand onto $\mathcal{S}_{\mathbf{r}}$. This action is fulfilled by using the tensor truncation operator $T_{\mathcal{S}} : \mathbb{W}_{\mathbf{q},dL} \to \mathcal{S}$ defined by

$$A_0 \in \mathbb{W}_{\mathbf{q},dL}: \quad T_{\mathcal{S}} A_0 = \mathrm{argmin}_{T\in\mathcal{S}} \|A_0 - T\|_{\mathbb{W}_{\mathbf{q}}}. \tag{3.6}$$

The replacement of A_0 by its approximation in $\mathcal{S}$ is called the *tensor truncation* to $\mathcal{S}$ and denoted by $T_{\mathcal{S}} A_0$. In computational practice we apply the quasioptimal tensor truncation operator. Since the approximation procedure in the QTT-format is performed by SVD-based algorithm, we arrive at the following conclusion.

Proposition 3.5 *(Tensor truncation). (a) The operator $T_{\mathcal{S}} : \mathbb{W}_{\mathbf{q},dL} \to \mathcal{S} := TT[\mathbf{r}, dL]$ is well defined. (b) For given $A_0 \in TT[\mathbf{r}_0, dL] \subset \mathbb{W}_{\mathbf{q},dL}$, and $\mathbf{r} < \mathbf{r}_0$, the quasioptimal approximation $T_{\mathcal{S}} A_0$ can be computed by QR/SVD based algorithm in $O(qdLr_0^3)$ operations.*

3.4 Numerics: QTT tensor calculus, solving equations in $\mathbb{R}^d$

The following numerics illustrates the behavior of approximation error vs. the TT-rank of the dyadic folding approximation ($q = 2$) applied to different classes of function related vectors/tensors. We apply the MATLAB subroutines in [36] implementing the binary folding of vectors and the low rank TT approximation.

Recall that for any $q = 2, 3, ...$, the QTT-rank (or more precisely, QTT$_q$-rank) of the exponential and trigonometric vectors equals 1 and 2, respectively. Moreover, it can be proven that the Kronecker-TT rank of the diagonal matrices generated by the exponential and trigonometric vectors equals 1 and 2, respectively (see Lemma 3.2). Furthermore, the product of exponential and sin-functions in arbitrary frequency range has the QTT-rank equals to 2, as for the single sin-function.

$N \setminus \overline{r}$	$e^{-\alpha x^2}, \alpha = 0.1, 1, 10, 10^2$	$\frac{\sin(\alpha x)}{x}, \alpha = 1, 10, 10^2$	$1/x$	e^{-x}/x	$x, x^{10}, x^{1/10}$
2^{10}	3.2/2.8/2.8/2.2	4.0/4.7/5.5	4	3.5	1.9/2.7/3.9
2^{12}	3.1/2.9/2.9/2.6	3.8/4.8/5.6	4.2	3.8	1.9/2.6/3.9
2^{14}	2.9/2.8/2.8/2.8	3.6/4.7/5.5	4.2	3.8	1.9/2.5/3.9
2^{16}	2.8/2.7/2.8/2.8 (0.03)	3.6/4.5/5.4 (0.048)	4.2 (0.05)	5.3 (0.04)	1.9/2.4/3.9

Table 3.1: QTT$_2$-ranks of functional N-vectors on large grids, $N = 2^p$.

Tables 3.1 and 3.2, present numerical results on the binary (i.e., $q = 2$) quantics ε-approximation with $\varepsilon = 10^{-6}$, of the function related vectors/tensors corresponding to monomials and fractional power of x, as well as to the functions

$$\frac{1}{x_1 + ... + x_d}, \quad \frac{1}{\|x\|}, \quad \frac{e^{-\alpha\|x\|}}{\|x\|}, \quad e^{-\alpha\|x\|}, \quad \frac{\sin(\alpha\|x\|)}{\|x\|} \quad x \in \mathbb{R}^d.$$

For the following discussion, the average separation rank of the QTT-model, $\overline{r}$, is defined by

$$\overline{r}^2 := \frac{1}{d}\sum_{\ell=1}^{d} r_{\ell-1} r_\ell,$$

providing the complexity bound $\leq 2d\overline{r}^2 \log N$ on the binary QTT approximation. The CPU time (sec.) corresponding to the finest grid is given in the brackets (see Table 3.1). It scales linearly in the input vector size, N. Notice for comparison that the FFT(N) on finest grid requires $t_{FFT}(2^{16}) \approx 0.006$ sec., indicating that the low rank QTT_2 vector-transform to higher dimension $D = \log N$, is almost as fast as the FFT on the same vector size.

Table 3.2 represents the QTT_2-ranks of the functional $N \times N$-matrices generated by sampling over large equidistant grids on $[0,1]^2$, approximated up to the tolerance $\varepsilon = 10^{-6}$. Here Δ_d denotes the d-Laplacian as in (3.1). The matrix notation $diag(e^{-x^2})$ means the diagonal matrix built by the N-vector generated by e^{-x^2} on the uniform grid. Approximation properties are similar in the case $d \geq 3$. The above numerical illustrations lead to the following promising observations.

$N \setminus \overline{r}$	$1/(x_1+x_2)$	$e^{-\|x\|}$	$e^{-\|x\|^2}$	$diag(e^{-x^2})$	$\Delta_2^{-1}\mathbf{1}, \varepsilon = 10^{-6}, 10^{-7}, 10^{-8}$
2^9	5.0	9.4	7.8	3.8	3.6/3.6/3.6
2^{10}	5.1	9.4	7.7	3.9	3.6/3.6/3.6
2^{11}	5.2	9.3	7.5	3.9	3.7/3.7/3.7

Table 3.2: QTT_2-ranks of functional $N \times N$-matrices on large grids, $N = 2^p$.

- The QTT-rank remains almost independent on the vector/matrix size, hence being specified only by analytic properties of generating function.
- The QTT-rank of the discrete Gaussians and monomials is very small (≤ 3), that means that any M-term exponential or polynomial expansion on large N-grid can be represented within the storage $O(M \log N)$.
- Vectors generated by singular functions like $1/x, e^{-x}/x$, $\sin(\alpha x)/x$, and x^α, $(\alpha > 0)$ exhibit almost the same QTT-rank as smooth (analytic) functions, uniformly in the grid size N.

The last examples given in Table 3.3 illustrates the low TT-rank quantics approximability of the Newton potential $1/\|x\|$, in $\mathbb{R}^3$, the electron density $\rho(x)$, $x \in \mathbb{R}^3$, and the Hartree potential, $V_H := 1/\|x\| * \rho$, of CH_4 molecule discretised over large $N \times N \times N$ spatial grid, and computed in [28] by the multigrid Tucker-canonical decomposition. In all cases the approximation accuracy $\varepsilon = 10^{-6}$ in the QTT-format is achieved. In Table 3.3, Hart(S) and Hart(F) correspond to the middle $N \times N$ matrix slice and to the full $N \times N \times N$-array representing the discrete Hartree potential, respectively.

N	$1/\|x\|$	$\rho(x)$	Hart(S)	Hart(F)
128	13.8	32.0	13.7	32.1
256	16.0	40.0	14.2	34.9
512	17.5	45.8	14.2	20.2
1024	18.0	48.6	13.9	28.2

N	V_3	$V_1 \times V_2 \times V_3$
128	2.8	2.8
256	3.0	3.0
512	3.3	3.3
1024	3.5	3.5

Table 3.3: QTT_2-ranks of $1/\|x\|$, the Hartree potential, and electron density of CH_4 (left); QTT_2-ranks for the canonical vectors of electron density of CH_4 (right).

We conclude that QTT-ranks of the Newton and Hartree potentials are rather small and remain almost uniformly bounded in N ($O(\log N)$ scaling). In turn, the QTT rank of the electron density ρ, has the tendency to approach the canonical rank of the respective discrete density $N \times N \times N$-tensor.

For comparison, Table 3.3 gives typical QTT ranks of the canonical-TT representation in $\mathcal{C}_{R,\mathbf{n}}[TT[\mathbf{r}, \log N]]$. Here V_k, $(k = 1, 2, 3)$ denote the canonical vectors of the leading term in the rank-R canonical representation of the electron density of CH_4 molecule. Table 3.3 (right) indicates that in the case of electron density tensor of CH_4 molecule (the canonical ε-rank is about $R \approx 50$ for $\varepsilon = 10^{-6}$), the two-level $\mathcal{C}_{R,\mathbf{n}}[TT[\mathbf{r}, \log N]]$-representation provides some better compression rate than those for the complete QTT approximation (cf. Table 3.3).

Table 3.4 represents the average QTT-ranks in approximation of certain function related matrices up to fixed tolerance $\varepsilon = 10^{-5}$. Among others, it includs the important example of matrix exponential (cf. Conjecture 3.3). In all cases, one can observe that rank parameters are small, and depend very mildly on the grid size.

$N \setminus \overline{r}$	$e^{-\alpha\Delta_1}, \alpha = 0.1, 1, 10, 10^2$	Δ_1^{-1}	$diag(1/x^2)$	$diag(e^{-x^2})$
2^9	6.2/6.8/9.7/11.2	6.2	5.1	4.0
2^{10}	6.3/6.8/9.5/10.8	6.3	5.3	4.0
2^{11}	6.4/6.8/9.0/10.4	6.2	5.5	4.1

Table 3.4: QTT_2-matrix-ranks of $N \times N$-matrices for large $N = 2^p$.

In Table 3.5, we present the average QTT_2-ranks of the finite difference solution of the Poisson equation in the unite cube in $\mathbb{R}^d$, up to the tolerance $\varepsilon = 10^{-5}$,

$$\Delta_d U = F \in \mathbb{R}^{N\times\ldots\times N}, \quad \text{on large} \quad N \times \ldots \times N \quad \text{uniform } d\text{-dimensional grid}$$

with $N = 2^p$, and for $d = 25, 50, 100, 200$. We consider the case $F = 1$, that corresponds to the nonseparable solution with weak singularities at the adge and corner points, requiring large spacial grids to provide higher resolution. The CPU time (sec.) is presented, that does not count the (problem independent) preprocessing cost required to compute the QTT_2 representation of $1D$ matrix exponentials, $\{\exp(-t_k\Delta_1)\}$, $t_k > 0$, $k = -M, ..., M$, of size $N \times N$ (the latter can be precomputed once and stored).

$N \setminus d$	25		50		100		200	
	r	$time$	r	time	r	time	r	time
2^7	10.0	0.0124	8.0	0.023	7.8	0.047	5.2	0.089
2^8	10.1	0.015	8.2	0.026	6.4	0.05	5.1	0.1
2^9	10.2	0.016	8.2	0.03	6.4	0.06	5.1	0.12
2^{10}	10.2	0.0177	8.4	0.03	6.4	0.061	5.0	0.127

Table 3.5: QTT_2-ranks for solution of the Poisson equation in $\mathbb{R}^d$ on large grids, $N = 2^p$.

One observes the systematic decay of the average rank parameter $\overline{r}$, in the growing dimension d, with stabilization to the small value about several ones. It is worth to note that the CPU computing time increases only logarithmically in the grid size N and linearly in d, as predicted by the theory: The total numerical cost is estimated by $O(d \log \varepsilon^{-1} \log N)$.

For the loading vector F, corresponding to the R-term sum of trigonometric functions the QTT-rank is estimated by $r \le R$, again leading to the log-log computational cost $O(dR \log \varepsilon^{-1} \log N)$.

4 Conclusions

We present the $O(d \log N)$-complexity quantics approximation method applied to high-order N-d tensors arising as the grid representation of physically relevant functions and operators in $\mathbb{R}^d$. The quantics method is based on the folding of initial N-d tensor to the auxiliary higher dimensional space of q-D tensors with $D = d \log_q N$ and $q = 2, 3$. The rigorous analysis on the low-rank quantics tensor approximation in the classes of function related N-d arrays, indicates the log-log scaling, $O(d \log \varepsilon^{-1} \log N)$, in both the grid size and numerical precision $\varepsilon > 0$. In particular, we prove the uniform canonical and QTT rank estimates for exponential, trigonometric and polynomial sampling representations, with implication to wavelet besis functions. Using the so-called QTT (or more generally, QTC) format, the nonlinear quantics tensor approximation can be implemented on the base of stable, noniterative QR/SVD algebraic decompositions with controlled accuracy $\varepsilon > 0$.

The QTT approximation method can be applied in the framework of truncated iteration for solving certain classes of elliptic/parabolic equations in higher dimensions with log-scaling in the basic discretisation parameters[2]. Extensive numerical tests in §3.4 illustrate the high compression rate provided by the quantics method applied to data arrays arising in the traditional FEM calculations and in computational quantum chemistry (see also [30, 31]).

We hope that the quantics-TC numerical method opens new perspectives for developing reliable computational schemes in higher dimensions that are free of the "curse of dimensionality", noticeable limitations on the univariate grid-size, and from numerical instabilities.

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