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Abstract

The aim of this paper is to construct explicit tensor-train representations for certain function-related tensors and vectors, which are constructed on the basis of introduced *functional tensor train decomposition*. These results are then used to construct explicit quantics tensor train decomposition for polynomial and sine functions.

1. Introduction

The aim of this paper is to provide explicit expressions for certain TT(*tensor train*)-decompositions of function-related tensors. TT-decomposition (or TT-approximation) for a d-dimensional tensor $\mathbf{A} = [A(i_1, i_2, \dots, i_d)], 1 \leqslant i_k \leqslant n_k$, is defined as [8]

$$A(i_1, i_2, \dots, i_d) \approx \sum_{\alpha_1, \dots, \alpha_{d-1}} G_1(i_1, \alpha_1) G_2(\alpha_1, i_2, \alpha_2) \dots G_d(\alpha_{d-1}, i_d), \tag{1}$$

where auxiliary indices α_k vary from 1 to r_k. Numbers r_k are called *compression ranks* or simply *TT-ranks*. In multilinear algebra there are two standard decompositions: *canonical decomposition* (or canonical approximation in non-exact case) [1, 2] and Tucker decomposition [3]. For more details on properties of canonical and Tucker decompositions, see recent review [4]. Canonical decomposition has form

$$A(i_1, i_2, \dots, i_d) \approx \sum_{\alpha=1}^{r} U_1(i_1, \alpha) \cdot \dots \dots \cdot U_d(i_d, \alpha). \tag{2}$$

Computation of this decomposition is an NP-hard problem, and moreover the approximation problem can be ill-posed [5]. There is another decomposition, called *Tucker decomposition* which has form

$$A(i_1, i_2, \dots, i_d) \approx \sum_{\alpha_1, \dots, \alpha_d} G(\alpha_1, \dots, \alpha_d) U_1(i_1, \alpha_1) \dots U_d(i_d, \alpha_d). \tag{3}$$

Quasioptimal Tucker approximation can be computed utilizing matrix singular value decomposition (SVD) [6, 7].

TT-decomposition (1) is in the middle between these two. If the canonical decomposition (or approximation) with rank r exists, there exists TT-decomposition with ranks $r_k \leqslant r$, and no more than dnr^2 memory cells, where $n = \max n_k$ are required. There is no exponential dependence from d, but the decomposition can be computed in a stable way using d sequential SVD [8]. Ranks r_k can be computed as ranks of *unfolding matrices*:

Theorem 1. *For a tensor* $\mathbf{A}$ *there exists TT-decomposition with ranks*

$$r_k = \operatorname{rank} A_k, \quad A_k = A(i_1 i_2 \dots i_k; i_{k+1} \dots i_d), \tag{4}$$

i.e. first k indices of A enumerate rows of A_k, and last $(d-k)$ — columns of it. In MATLAB in can be realized as one reshape operation:

$$A_k = \text{reshape}(A, \prod_{s=1}^{k} n_s, \prod_{s=k+1}^{d} n_s).$$

Therefore, computation of compression ranks is reduced to the computation of matrix ranks, and this can be done (in principle) by Gaussian elimination in finite amount of operations (compared to the NP-hard problem of computing canonical rank). The proof of Theorem 1 is constructive and is based on simple successive separation of indices. First, separate i_1 using any dyadic decomposition:

$$A(i_1, \ldots, i_d) = \sum_{\alpha_1=1}^{r_1} G_1(i_1, \alpha_1) V(\alpha_1 i_2, i_3, \ldots, i_d).$$

It can be shown, that if $\mathbf{V} = V(\alpha_1 i_2, i_3, \ldots, i_d)$ is considered as $(d-1)$-dimensional tensor with $(\alpha_1 i_2)$ as "long" first mode index, then ranks of its unfoldings $V_2, \ldots, V_d$ are not larger than $r_2, \ldots r_d$ defined in (4), so $(\alpha_1 i_2)$ can be separated:

$$V(\alpha_1 i_2, i_3, \ldots, i_d) = \sum_{\alpha_2=1}^{r_2} G_2(\alpha_1, i_2, \alpha_2) W(\alpha_2 i_3, \ldots, i_d),$$

which gives the second core $G_2(\alpha_1, i_2, \alpha_2)$. The procedure is then applied to tensor W and so on. Complexity of this algorithm (called TT-SVD) is estimated as $\mathcal{O}(Nr^2)$, where $N = n_1 n_2 \ldots n_d$ is the number of elements in the tensor. Of course, this algorithm requires full array to be stored and it does not avoid the curse of dimensionality. However, it can be used as a basis for fast adaptive algorithms. If a tensor is already in a structured format (TT-format with non-optimal ranks, canonical format) it can be implemented fast using *recompression* [8]. For a general black-box tensor TT-cross algorithm can be used [9].

From numerical point of view TT-decomposition is very suitable, and if it is known that decomposition exists, it can be computed robustly. However, theoretical estimates for ranks and explicit representations for some classes of tensors are not yet well developed. In this paper we focus on function-related tensors, that appear in two cases. The fist one is the most obvious. Elements of a tensor are values of a multivariate function on a tensor grid:

$$A(i_1, i_2, \ldots, i_d) = f(x_1(i_1), x_2(i_2), \ldots, x_d(i_d)), \quad 1 \leqslant i_k \leqslant n_k, k = 1, \ldots, d, \tag{5}$$

where $x_k(i_k)$ are some one-dimensional grids. There is direct connection between *canonical decomposition* and *separated representation of functions*: if

$$f(x_1, \ldots, x_d) = \sum_{\alpha=1}^{r} g_1(x_1, \alpha) g_2(x_2, \alpha) \ldots g_d(x_d, \alpha),$$

then tensor $\mathbf{A}$ defined by (5) has canonical rank r. Indeed, the only difference is that the discrete index i_k is replace by continuos variable x_k, thus any estimate of the separation rank r gives an upper bound for a function-related tensor $\mathbf{A}$. In this paper we investigate this connection for the TT-decomposition and introduce continuos analogue of TT-decomposition for functions — *functional TT-decomposition*, or FTT. It appears that for several important functions it is not difficult to obtain explicit FTT representation (and thus, TT-representation of their function-related tensor), and that is done in this paper.

The second case are tensors, obtained from *quantics tensor train representation* (QTT) of "low-dimensional" functions. Consider univariate function, $f(x)$, defined on an interval $[a, b]$, and introduce uniform grid $[x_k], k = 1, \dots, n$ with $n = 2^d$ points, and a vector v of values of the function on this grid:

$$v_k = f(x_k).$$

This vector can be reshaped (or tensorized) into a $2 \times 2 \times \dots \times 2$ d-dimensional tensor. In MATLAB, it can be done by command

$$\mathbf{V} = \mathrm{reshape}(v, 2{*}\mathrm{ones}(1{,}d)).$$

For this tensor, TT-decomposition (or TT-approximation) is computed. QTT was introduced in [10] in the context of tensorization of matrices, and then studied by Khoromskij [11] for vectors, where it was shown that for

$$f(x) = e^{\lambda x},$$

corresponding tensor has canonical rank 1 (thus, all TT-ranks are equal to 1), and for the function

$$f(x) = \sin \omega x,$$

TT-ranks are equal to 2.[1] Numerical experiments also confirm, that for many functions (including functions with point singularities) TT-ranks for tensorized vector (or simply QTT-ranks) remain small and depend logarithmically on the accuracy of the approximation ε.

Since estimation of TT-ranks is reduced to the estimation of ranks of unfolding matrices, it is sometimes not difficult to obtain estimates for these ranks. Grasedyck [12] proved that for polynomials, $p(x) = x^k$, ranks are bounded by $(k + 1)$. However, such estimates do not lead to explicit TT-representations (except for the exponential case). The goal of the paper is to fill this gap and present explicit TT (and QTT) decompositions of several function-related tensors and vectors.

2. Functional TT-decomposition and explicit formulae for certain functions

2.1. Functional TT-decomposition

As separated representation of a function is a continuos analogue of the canonical decomposition of a tensor, there is a simple generalization of the TT-decomposition to functions. It has the same form as (1), but with discrete indices i_k replaced by continuos variables x_k:

$$f(x_1, \dots, x_d) \approx \sum_{\alpha_1, \dots, \alpha_{d-1}} g_1(x_1, \alpha_1) g_2(\alpha_1, x_2, \alpha_2) \dots g_d(\alpha_{d-1}, x_d). \tag{6}$$

[1] Canonical ranks depend on the field: for complex numbers rank is equal to 2, but for real it seems to be d, however, no proof is available.

This decomposition can be rewritten in a compact form (the discrete variant is described in [8]):

$$f(x_1, \dots, x_d) \approx g_1(x_1)G_2(x_2)G_3(x_3)\dots G_{d-1}(x_{d-1})g_d(x_d), \tag{7}$$

where $g_1(x_1)$ is a column vector function, $G_k(x_k)$ is a matrix, depending on x_k (matrix has size $r_{k-1} \times r_k$ and its elements depend on x_k), and, finally, g_d is a row vector function (or matrix of size $r_{d-1} \times 1$). Thus, the function is represented (or approximated) by a product of matrices, and each matrix depends only on one variable. The form (7) is usually the most compact one form of functional tensor train decompostion.

2.2. FTT for a special polynomial function

In several cases it is possible to write down TT-decomposition explicitly, and we will show how it can be done. Let us start from the function

$$f(x_1, \dots, x_d) = x_1 + \dots + x_d. \tag{8}$$

It was considered in [13, 14]. It can be shown, that this function can be approximated by separable rank-2 approximation with any required accuracy, but no exact rank-2 approximation exists. It follows from the formula

$$x_1 + \dots + x_d = \frac{\prod_{s=1}^{d}(1+\varepsilon x_s) - 1}{\varepsilon} + \mathcal{O}(\varepsilon),$$

and ε can be chosen as small as required. The problems are on numerical side: after discretization, norms of canonical factors will grow, and the approximation is due to subtraction of two large numbers. Thus, since all computations are possible only up to machine precision, the rank is dependent on it (logarithmically). For details, see [13, 14]. However, since the set of matrices of fixed rank is closed, it immediately follows that all TT-ranks for this example (on the discrete level) are equal to 2. On the continuos level the same is true, and can be proven using the same arguments. However, we will just provide an explicit FTT-representation for this example. The final result is very simple and easy to check directly: but to illustrate the idea, we will obtain it constructively.

Let us start separation of variables, as in TT-SVD algorithm. First, separate x_1:

$$f(x) = \begin{pmatrix} x_1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ x_2 + \dots + x_d \end{pmatrix}$$

Now, x_2 has to be separated. Instead of one function, we have one vector function with two components. Each of these can depend on x_2. Suppose the general case: vector function has form

$$\begin{pmatrix} h_1(x_2, \dots, x_d) \\ h_2(x_2, \dots, x_d) \end{pmatrix}$$

If x_2 can be separated with r_{21} terms in h_1, and r_{22} in h_2, then r_2 is not greater that $r_{21} + r_{22}$. However, if in expansions

$$h_1(x_2, \dots, x_d) = \sum_{\alpha=1}^{r_{21}} \varphi_\alpha(x_2) H_\alpha^{(1)}(x_3, \dots, x_d),$$

$$h_2(x_2,\ldots,x_d) = \sum_{\beta=1}^{r_{22}} \psi_\beta(x_2) H^{(2)}_\alpha(x_3,\ldots,x_d),$$

functions φ_α, φ_β are not linearly independent and the dimension of their linear span is equal to r, then r_2 is equal to r, since vector function can be written as

$$\begin{pmatrix} h_1(x_2,\ldots,x_d) \\ h_2(x_2,\ldots,x_d) \end{pmatrix} = \Psi(x_2) H(x_3,\ldots,x_d),$$

where matrix Ψ is $2\times r$ and H is a column vector of length r. For the particular function,

$$h_1 = 1, \quad h_2 = x_2 + 1 \cdot (x_3 + \ldots + x_d),$$

i.e. there are two basis functions: 1 and x_2 and r_2 is equal to 2. The next step of the decomposition reads

$$\begin{pmatrix} 1 \\ x_2 + \ldots + x_d \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ x_2 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ x_3 + \ldots + x_d \end{pmatrix}$$

Continuing this process, we obtain explicit decomposition for function (8). It is clear from previous considerations, that everything works also for functions of form

$$f(x_1,\ldots,x_d) = w_1(x_1) + w_2(x_2) + \ldots + w_d(x_d),$$

where $w_k(x_k)$ are arbitrary one-dimensional functions. The results are summarized in Theorem 2.

Theorem 2. *For a function*

$$f(x_1,\ldots,x_d) = w_1(x_1) + w_2(x_2) + \ldots + w_d(x_d),$$

TT-decomposition has form

$$f = \begin{pmatrix} w_1(x_1) & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ w_2(x_2) & 1 \end{pmatrix} \cdot \ldots \cdot \begin{pmatrix} 1 & 0 \\ w_{d-1}(x_{d-1}) & 1 \end{pmatrix} \begin{pmatrix} 1 \\ w_d(x_d) \end{pmatrix}$$

When the explicit expression is obtained, it becomes trivial, since for any a and b

$$\begin{pmatrix} 1 & 0 \\ a & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ b & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ a+b & 1 \end{pmatrix}.$$

The same idea can be used to get FTT decomposition for a function of form

$$f(x_1,\ldots,x_d) = M(x_1 + \ldots + x_d), \tag{9}$$

where $M(z)$ is a polynomial of degree p:

$$M(z) = \sum_{k=0}^{p} a_k z^k.$$

First, separate x_1. Note, that for any x, y

$$M(x+y) = \sum_{k=0}^{q} a_k (x+y)^k = \sum_{k=0}^{p} a_k \sum_{s=0}^{k} C_k^s y^s x^{k-s} = \sum_{s=0}^{p} y^s \sum_{k=s}^{p} C_k^s x^{k-s} = \sum_{s=0}^{p} y^s \varphi_s(x),$$

where

$$\varphi_s(x) = \sum_{k=s}^{p} a_k C_k^s x^{k-s},$$

and C_k^s is the binomial coefficient:

$$C_k^s = \frac{k!}{s!(k-s)!}.$$

Therefore

$$f = g_1(x_1) \begin{pmatrix} 1 \\ (x_2 + \ldots + x_d) \\ (x_2 + \ldots + x_d)^2 \\ \vdots \\ (x_2 + \ldots + x_d)^p \end{pmatrix},$$

and the first rank is $r_1 = (p+1)$. As for the second rank, for each element of the vector function separation of x_2 is done as

$$(x_2 + \ldots + x_d)^k = \sum_{s=0}^{k} C_k^s x_2^s (x_3 + \ldots + x_d)^{k-s},$$

and there are exactly $(p+1)$ basis functions: $1, x_2, \ldots, x_2^p$, and the matrix is represented as

$$f(x) = g_1(x_1) G_2(x_2) \begin{pmatrix} 1 \\ (x_3 + \ldots + x_d) \\ (x_3 + \ldots + x_d)^2 \\ \vdots \\ (x_3 + \ldots + x_d)^p \end{pmatrix},$$

where

$$G_2(x_2) = \begin{pmatrix} C_0^0 & 0 & \cdots & \cdots & \cdots & 0 \\ C_1^1 x_2 & C_1^0 & 0 & \cdots & \cdots & 0 \\ C_2^2 x_2^2 & C_2^1 x_2 & C_2^0 & \ddots & \cdots & 0 \\ C_3^3 x_2^3 & C_3^2 x_2^2 & C_3^1 x_2 & C_3^0 & \ddots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ C_p^p x_2^p & C_p^{p-1} x_2^{p-1} & \cdots & \cdots & C_p^1 x_2 & C_p^0 \end{pmatrix},$$

or

$$G_2(x_2)_{ij} = \begin{cases} C_i^{i-j} x_2^{i-j}, & i \geqslant j \\ 0, & i < j \end{cases}, \quad i, j = 0, \ldots, p.$$

Since the remaining vector has the same form, all other matrices $G_k(x_k)$ will have the same form. The last core of the FTT decomposition (which is a column vector) is simply

$$g_d(x_d) = \begin{pmatrix} 1 \\ x_d \\ x_d^2 \\ \vdots \\ x_d^p \end{pmatrix}.$$

The results are summarized in Theorem 3.

Theorem 3. *For a function*

$$f(x_1, \ldots, x_d) = M(x_1 + \ldots + x_d),$$

where $M(z)$ is degree-p polynomial,

$$M(z) = \sum_{k=0}^{p} a_k z^k,$$

FTT decomposition has form

$$f = g_1(x_1)G(x_2)G(x_3)\ldots G(x_{d-1}g_d(x_d),$$

where $G(x)$ is matrix function of size $(p+1) \times (p+1)$ with elements

$$G(x)_{ij} = \begin{cases} C_i^{i-j} x_2^{i-j}, & i \geqslant j \\ 0, & i < j \end{cases}, \quad i, j = 0, \ldots, p,$$

and

$$\begin{aligned} g_1(i_1) &= \begin{pmatrix} \varphi_0(x_1) & \varphi_1(x_1) & \cdots & \varphi_{p-1}(x_1) & \varphi_p(x_1) \end{pmatrix}, \\ \varphi_s(x) &= \sum_{k=s}^{p} a_k C_k^s x^{k-s}, \quad s = 0, \ldots, p \end{aligned}$$

and

$$g_d(x_d) = \begin{pmatrix} 1 \\ x_d \\ x_d^2 \\ \vdots \\ x_d^p \end{pmatrix}.$$

2.3. FTT for a sine of a sum

Another example, considered in previous works [15, 13, 14] is the sine of a sum:

$$f(x_1, \dots, x_d) = \sin(x_1 + x_2 + \dots + x_d). \tag{10}$$

In the complex field, due to the equality

$$\sin x = \frac{e^{ix} - e^{-ix}}{2i},$$

the separation rank is equal to 2. In the real field, using simple trigonometric identities, it is possible to obtain estimate $r \leqslant 2^{d-1}$. In [13] decomposition with $r = d$ terms was presented, and it seems to be the best possible for the canonical rank. However, TT-ranks are equal to 2, since they are ranks of unfolding matrices, and matrix rank is the same over real and complex fields. In this paper we will present an explicit FTT decomposition for the function (10).

The idea of the proof is the same. First, separate x_1 using well-known trigonometric identity:

$$\begin{aligned} f &= \sin x_1 \cos(x_2 + \dots + x_d) + \cos x_1 \sin(x_2 + \dots + x_d) = \\ &= \begin{pmatrix} \sin x_1 & \cos x_1 \end{pmatrix} \begin{pmatrix} \cos(x_2 + \dots + x_d) \\ \sin(x_2 + \dots + x_d) \end{pmatrix}. \end{aligned}$$

Now, separate x_2 in each element of the vector function:

$$\begin{aligned} \cos(x_2 + \dots + x_d) &= \cos x_2 \cos(x_3 + \dots + x_d) - \sin x_2 \sin(x_3 + \dots + x_d), \\ \sin(x_2 + \dots + x_d) &= \sin x_2 \cos(x_3 + \dots + x_d) + \cos x_2 \sin(x_3 + \dots + x_d), \end{aligned}$$

Therefore,

$$\begin{pmatrix} \cos(x_2 + \dots + x_d) \\ \sin(x_2 + \dots + x_d) \end{pmatrix} = \begin{pmatrix} \cos x_2 & -\sin x_2 \\ \sin x_2 & \cos x_2 \end{pmatrix} \begin{pmatrix} \cos(x_3 + \dots + x_d) \\ \sin(x_3 + \dots + x_d) \end{pmatrix},$$

and the process continues further on in the same way. The final result is summarized in Theorem 4.

Theorem 4. *For a function*

$$f(x_1, \dots, x_d) = \sin(x_1 + x_2 + \dots + x_d),$$

FTT decomposition has form

$$f = \begin{pmatrix} \sin x_1 & \cos x_1 \end{pmatrix} \begin{pmatrix} \cos x_2 & -\sin x_2 \\ \sin x_2 & \cos x_2 \end{pmatrix} \cdot \ldots \cdot \begin{pmatrix} \cos x_{d-1} & -\sin x_{d-1} \\ \sin x_{d-1} & \cos x_{d-1} \end{pmatrix} \begin{pmatrix} \cos x_d \\ \sin x_d \end{pmatrix}.$$

Note, that matrices $G_k(x_k)$ for this decomposition are orthogonal, which can is important for numerical stability.

2.4. FFT for a Hankel function

Two previous results, giving a closed form for the FFT decomposition, can be generalized to the case of *Hankel functions*. Consider function that depends on the sum of $x_1 + \ldots + x_d$:

$$f = H(x_1 + x_2 + \ldots + x_d).$$

It is possible to get explicit FTT representations for such kind of functions? Suppose that $H(x+y)$ has separation rank r:

$$H(x+y) = \sum_{\alpha=1}^{r} u_\alpha(x) v_\alpha(y),$$

and functions $u_\alpha(x)$ and $v_\alpha(y)$ form two linearly independent sets.

Then, due to functional skeleton decomposition [16], there exist points $\widehat{x}_i, i = 1, \ldots, r$, $\widehat{y}_j, j = 1, \ldots, r$, such that

$$H(x+y) = \sum_{i,j=1}^{r} H(x + \widehat{y}_i) M_{ij} H(\widehat{x}_j + y), \tag{11}$$

where

$$[M_{ij}] = [H(\widehat{x}_i + \widehat{y}_j)]^{-1}.$$

The only requirement for (11) to be true is that nodes $\widehat{x}_i$ and $\widehat{y}_j$ are chosen so that matrix

$$[H(\widehat{x}_i + \widehat{y}_j)]$$

is nonsingular. Let us write it in form

$$H(x+y) = \sum_{i=1}^{r} H(\widehat{y}_i + x) \psi_i(y), \tag{12}$$

where

$$\psi_i(y) = \sum_{j=1}^{r} M_{ij} H(\widehat{x}_j + y)$$

Now, let us start construction of FTT decomposition for a function f. From (11),(12) it follows that

$$f = \begin{pmatrix} \psi_1(x_1) & \psi_2(x_1) & \cdots & \psi_r(x_1) \end{pmatrix} \begin{pmatrix} H(\widehat{y}_1 + (x_2 + \ldots + x_d)) \\ H(\widehat{y}_2 + (x_2 + \ldots + x_d)) \\ \vdots \\ H(\widehat{y}_r + (x_2 + \ldots + x_d)) \end{pmatrix}.$$

For each element of this vector, x_2 can be now separated:

$$H(\widehat{y}_k + (x_2 + \ldots + x_d)) = \sum_{i=1}^{r} \psi_i(\widehat{y}_k + x_2) H(\widehat{y}_i + (x_3 + \ldots + x_d)),$$

therefore

$$\begin{pmatrix} H(\widehat{y}_1 + (x_2 + \ldots + x_d)) \\ H(\widehat{y}_2 + (x_2 + \ldots + x_d)) \\ \vdots \\ H(\widehat{y}_r + (x_2 + \ldots + x_d)) \end{pmatrix} = G_2(x_2) \begin{pmatrix} H(\widehat{y}_1 + (x_3 + \ldots + x_d)) \\ H(\widehat{y}_2 + (x_3 + \ldots + x_d)) \\ \vdots \\ H(\widehat{y}_r + (x_3 + \ldots + x_d)) \end{pmatrix},$$

where G_2 is $r \times r$ matrix with elements

$$G_2(x_2)_{ij} = \psi_i(x_2 + \widehat{y}_j).$$

The results are summarized in Theorem 5

Theorem 5. *Let* f *be a function that depends on a sum of arguments:*

$$f(x_1, \ldots, x_d) = H(x_1 + x_2 + \ldots + x_d),$$

where function $H(x + y)$ *has separation rank* r. *Then*

1. *All FTT-ranks are bounded by* r.

2. *If, additionally,* $\widehat{x}_i, i = 1, \ldots, r$ *and* $\widehat{y}_j, j = 1, \ldots, r$ *are known such that matrix with elements* $H(\widehat{x}_i + \widehat{y}_j)$ *is nonsingular, then FTT decomposition has form*

$$f = g_1(x_1) G(x_2) \cdot \ldots \cdot G(x_{d-1}) g_d(x_d),$$

where

$$\begin{aligned} g_1(x_1) &= \begin{pmatrix} \psi_1(x_1) & \psi_2(x_1) & \cdots & \psi_r(x_1) \end{pmatrix}, \\ G(x)_{ij} &= \psi_i(x + \widehat{y}_j), \\ \psi_i(z) &= \sum_{j=1}^{r} M_{ij} H(\widehat{x}_j + z), \\ g_d(x_d) &= \begin{pmatrix} H(\widehat{y}_1 + x_d) \\ H(\widehat{y}_2 + x_d) \\ \vdots \\ H(\widehat{y}_r + x_d) \end{pmatrix}, \end{aligned}$$

and

$$[M_{ij}] = [H(\widehat{x}_i + \widehat{y}_j)]^{-1}.$$

3. Quantics TT-decomposition of certain functions

In this section we will use results of Section 2 to get explicit QTT decompositions of certain functions.

Theorem 6. *Let* $M(x) = \sum_{k=0}^{p} a_k x^k$ *be a polynomial of degree* p *on an interval* $[a, b]$. *Consider uniform grid on this interval:*

$$x_i = a + ih, h = \frac{b-a}{n-1}, n = 2^d,$$

and vector

$$v_i = M(x_i),$$

and tensor $2 \times 2 \times \ldots \times 2$ *tensor* $\mathbf{V}$ *which is a reshape of* v*:*

$$V(i_1, i_2, \ldots, i_d) = v(i),$$

where $i_k \in \{0, 1\}$ *are binary digits of integer* i. *Then, TT-decomposition of* $\mathbf{V}$ *has form (and QTT-decomposition of of* $M(x)$*)*

$$V(i_1, i_2, \ldots, i_d) = g_1(i_1) G_2(i_2) \ldots G_{d-1}(i_{d-1}) g_d(i_d),$$

where

$$\begin{aligned}
g_1(i_1) &= \begin{pmatrix} \varphi_0(\frac{a}{d} + i_1 h) & \varphi_1(\frac{a}{d} + i_1 h) & \cdots & \varphi_{p-1}(\frac{a}{d} + i_1 h) & \varphi_p(\frac{a}{d} + i_1 h) \end{pmatrix}, \\
\varphi_s(x) &= \sum_{k=s}^{p} a_k C_k^s x^{k-s}, \quad s = 0, \ldots, p \\
G_k(i_k) &= G(\frac{a}{d} + 2^k i_k h), \\
G(x)_{ij} &= \begin{cases} C_i^{i-j} x^{i-j}, & i \geqslant j \\ 0, & i < j \end{cases}, \quad i, j = 0, \ldots, p \\
g_d(i_d) &= g(\frac{a}{d} + 2^d i_d h), \\
g(x) &= \begin{pmatrix} 1 \\ x \\ x^2 \\ \vdots \\ x^p \end{pmatrix}.
\end{aligned}$$

Proof. To prove the Theorem, it is sufficient to note that

$$V(i_1, i_2, \ldots, i_d) = v(i) = v(i_1 + 2i_2 + 4i_3 + \ldots 2^{d-1} i_d) = M(x_1 + x_2 + \ldots + x_d),$$

where $x_k = 2^{k-1} i_k h + \frac{a}{d}$, and apply Theorem 3.

For the sine function we have the following

Theorem 7. *Let* $f(x) = \sin x$, *and interval* $[a, b]$. *Consider uniform grid on this interval:*

$$x_i = a + ih, h = \frac{(b-a)}{n-1}, n = 2^d,$$

and vector

$$v_i = f(x_i),$$

and tensor $2 \times 2 \times \ldots \times 2$ *tensor* $\mathbf{V}$ *which is a reshape of* v*:*

$$V(i_1, i_2, \ldots, i_d) = v(i),$$

where $i_k \in \{0, 1\}$ *are binary digits of integer* i*. Then, TT-decomposition of* $\mathbf{V}$ *has form*

$$\begin{aligned} V(i_1, i_2, \ldots, i_d) &= \begin{pmatrix} \sin x_1 & \cos x_1 \end{pmatrix} \begin{pmatrix} \cos x_2 & -\sin x_2 \\ \sin x_2 & \cos x_2 \end{pmatrix} \cdot \ldots \\ & \ldots \cdot \begin{pmatrix} \cos x_{d-1} & -\sin x_{d-1} \\ \sin x_{d-1} & \cos x_{d-1} \end{pmatrix} \begin{pmatrix} \cos x_d \\ \sin x_d \end{pmatrix}, \\ \text{where } x_k &= \frac{a}{d} + 2^{k-1} i_k h. \end{aligned}$$

Proof. To prove the Theorem, it is sufficient to note that

$$V(i_1, i_2, \ldots, i_d) = v(i) = v(i_1 + 2i_2 + 4i_3 + \ldots 2^{d-1} i_d) = \sin(x_1 + x_2 + \ldots + x_d),$$

where $x_k = \frac{a}{d} + 2^{k-1} i_k h$, and apply Theorem 4.

Finally, we extend result of Theorem 5 to the QTT format in a similar way.

Theorem 8. *Let* $f(x)$ *be a function defined on an interval* $[a, b]$ *and* $f(x+y)$ *has separation rank* r*. Consider uniform grid on this interval:*

$$x_i = a + ih, h = \frac{(b-a)}{n-1}, n = 2^d,$$

and vector

$$v_i = f(x_i),$$

and tensor $2 \times 2 \times \ldots \times 2$ *tensor* $\mathbf{V}$ *which is a reshape of* v*:*

$$V(i_1, i_2, \ldots, i_d) = v(i),$$

where $i_k \in \{0, 1\}$ *are binary digits of integer* i*. Then*

1. *All QTT-ranks are bounded by* r*.*
2. *If, additionally,* $\widehat{x}_i, i = 1, \ldots, r$ *and* $\widehat{y}_j, j = 1, \ldots, r$ *are known such that matrix with elements* $f(\widehat{x}_i + \widehat{y}_j)$ *is nonsingular, then TT decomposition of* $\mathbf{V}$ *(and QTT of* f*) has form*

$$V(i_1, i_2, \ldots, i_d) = g_1(x_1) G(x_2) \cdot \ldots \cdot G(x_{d-1}) g_d(x_d),$$

where

$$\begin{aligned}
g_1(x_1) &= \begin{pmatrix} \psi_1(x_1) & \psi_2(x_1) & \cdots & \psi_r(x_1) \end{pmatrix}, \\
G(x)_{ij} &= \psi_i(x+\widehat{y}_j), \\
g_d(x_d) &= \begin{pmatrix} f(\widehat{y}_1+x_d) \\ f(\widehat{y}_2+x_d) \\ \vdots \\ f(\widehat{y}_r+x_d) \end{pmatrix}, \\
\psi_i(z) &= \sum_{j=1}^{r} M_{ij} f(\widehat{x}_j+z), \\
x_k &= \frac{a}{d} + 2^{k-1} i_k h.
\end{aligned}$$

and

$$[M_{ij}] = [f(\widehat{x}_i+\widehat{y}_j)]^{-1},$$

Proof. To prove the Theorem, it is sufficient to note that

$$V(i_1, i_2, \ldots, i_d) = v(i) = v(i_1 + 2i_2 + 4i_3 + \ldots 2^{d-1} i_d) = f(x_1 + x_2 + \ldots + x_d),$$

where $x_k = \frac{a}{d} + 2^{k-1} i_k h$, and apply Theorem 5.

Corrolary 1. *For a rational function* $f(x) = \frac{p(x)}{q(x)}$, *where* p *and* q *are polynomials, defined on an interval* $[a, b]$, *and uniform grid with* $n = 2^d$ *grid points is used. Then, QTT-ranks behave logarithmically in accuracy* ε *of the QTT-approximation and number of grid points* n*:*

$$r_k = \mathcal{O}(\log^{\alpha} \varepsilon \log^{\beta} n). \tag{13}$$

Proof. Due to Theorem 8 QTT rank estimates are reduced to the estimation of the ε-separation rank of the function

$$g(x, y) = f(x + y).$$

For a rational function such estimates (which have required form (13)) can be obtained from results on the decay of singular values of Hankel operators [17, 18], and moreover such separable approximations can be constructed via constructive approximation schemes (for example, sinc-quadratures) [19].

4. Conclusion

In this paper we presented several explicit functional TT-decomposition of certain functions, which where unknown previously. Using these results, constructive representation of QTT decomposition of polynomials, sine function are obtained, and characterization of QTT-decomposition of a function f is given in terms of separation ranks of a function $f(x+y)$. These decomposition can be used as “building blocks” for constructing efficient algorithms working with function representations in these new formats.

References

[1] *Harshman R. A.* Foundations of the Parafac procedure: models and conditions for an explanatory multimodal factor analysis // *UCLA Working Papers in Phonetics*. 1970. V. 16. P. 1-84.

[2] *Carroll J. D., Chang J. J.* Analysis of individual differences in multidimensional scaling via n-way generalization of Eckart-Young decomposition // *Psychometrika*. 1970. V. 35. P. 283-319.

[3] *Tucker L. R.* Some mathematical notes on three-mode factor analysis // *Psychometrika*. 1966. V. 31. P. 279-311.

[4] *Kolda T. G., Bader B. W.* Tensor Decompositions and Applications // *SIAM Review*. 2009. V. 51, № 3. P. 455. http://link.aip.org/link/SIREAD/v51/i3/p455/s1\&Agg=doi.

[5] *de Silva V., Lim L.-H.* Tensor Rank and the Ill-Posedness of the Best Low-Rank Approximation Problem // *SIAM Journal on Matrix Analysis and Applications*. 2008. V. 30, № 3. P. 1084. http://link.aip.org/link/SJMAEL/v30/i3/p1084/s1\&Agg=doi.

[6] *De Lathauwer L., De Moor B., Vandewalle J.* A multilinear singular value decomposition // *SIAM Journal on Matrix Analysis and Applications*. 2000. V. 21, № 4. P. 1253. http://link.aip.org/link/SJMAEL/v21/i4/p1253/s1\&Agg=doi.

[7] *De Lathauwer L., De Moor B., Vandewalle J.* On the best rank-1 and rank-$(R_1, R_2, ..., R_N)$ approximation of higher-order Tensors // *SIAM Journal on Matrix Analysis and Applications*. 2000. V. 21, № 4. P. 1324. http://link.aip.org/link/SJMAEL/v21/i4/p1324/s1\&Agg=doi.

[8] *Oseledets I. V.* Compact matrix form of the d-dimensional tensor decomposition. 2009.

[9] *Oseledets I. V., Tyrtyshnikov E. E.* TT-cross approximation for multidimensional arrays // *Linear Algebra and its Applications*. 2010. — . V. 432, № 1. P. 70–88. http://linkinghub.elsevier.com/retrieve/pii/S0024379509003747.

[10] *Oseledets I. V.* Approximation of $2^d \times 2^d$ matrices using tensor decomposition // *SIAM Journal of Matrix Analysis and Applications*. 2010. V. 31, № 4. P. 2130–2145.

[11] *Khoromskij B. N.* $\mathcal{O}(d \log N)$-Quantics Approximation of Nd Tensors in High-Dimensional Numerical Modeling. 2009. http://en.scientificcommons.org/52484259.

[12] *Grasedyck L.* Polynomial Approximation in Hierarchical Tucker Format by Vector-Tensorization: Preprint 78. — Aachen: Aachen University, 2010. http://www.dfg-spp1324.de/download/preprints/preprint043.pdf.

[13] *Beylkin G., Mohlenkamp M. J.* Numerical operator calculus in higher dimensions. // *Proceedings of the National Academy of Sciences of the United States of America*. 2002. — . V. 99, № 16. P. 10246–51. http://www.pnas.org/cgi/content/abstract/99/16/10246.

[14] *Beylkin G., Mohlenkamp M. J.* Algorithms for Numerical Analysis in High Dimensions // *SIAM Journal on Scientific Computing*. 2005. V. 26, № 6. P. 2133. http://link.aip.org/link/SJOCE3/v26/i6/p2133/s1\&Agg=doi.

[15] *Oseledets I. V., Tyrtyshnikov E. E.* Breaking the curse of dimensionality, or how to use SVD in many dimensions // *SIAM Journal on Scientific Computing*. 2009. V. 31, № 5. P. 3744. http://link.aip.org/link/SJOCE3/v31/i5/p3744/s1\&Agg=doi.

[16] *Oseledets I. V.* Lower bounds for separable approximations of the Hilbert kernel // *Sbornik: Mathematics*. 2007. — . V. 198, № 3. P. 425–432. http://stacks.iop.org/1064-5616/198/i=3/a=A05?key=crossref.54007840c4ce70f72155caa1e429d3b5.

[17] *Widom H.* Hankel matrices // *Trans. Amer. Math. Soc.* 1966. V. 121, № 1. P. 1–35.

[18] *Laptev A. A.* Spectral behaviour of a certain class of integral operators // *Math. Notes*. 1974. V. 16, № 5. P. 1038–1043.

[19] *Hackbusch W., Khoromskij B. N.* Low-rank Kronecker-product Approximation to Multi-dimensional Nonlocal Operators. Part I. Separable Approximation of Multi-variate Functions // *Computing*. 2005. — . V. 76, №3-4. P. 177–202. http://www.springerlink.com/content/74v20851143034q1.