

Max-Planck-Institut
für Mathematik
in den Naturwissenschaften
Leipzig

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full-rank Fourier images

by

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Preprint no.: 45

2011



QTT-RANK-ONE VECTORS WITH QTT-RANK-ONE AND FULL-RANK FOURIER IMAGES

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July 18, 2011

Abstract. Quantics tensor train (QTT), a new data-sparse format for one- and multi-dimensional vectors, is based on a bit representation of mode indices followed by a separation of variables. A radix-2 recurrence, that lays behind the famous FFT algorithm, can be efficiently applied to vectors in the QTT format. If input and all intermediate vectors of the FFT algorithm have moderate QTT ranks, the resulted QTT-FFT algorithm outperforms the FFT for large vectors. It is instructive to describe a class of such vectors explicitly. We find all vectors that have QTT ranks one on input, intermediate steps and output of the FFT algorithm. We also give an example of QTT-rank-one vector that has the Fourier image with full QTT ranks. By numerical experiments we show that for certain rank-one vectors with full-rank Fourier images, the practical ε -ranks remain moderate for large mode sizes.

Keywords: Multidimensional arrays, quantics tensor train, Fourier transform, data-sparse formats

AMS classification: 15A23, 15A69, 65F99, 65T50.

1. Introduction

For multi-dimensional data, storage and complexity grow prohibitively with the dimension and structured low-parametric formats are necessary to make the computations feasible. Recently, a *tensor train* (TT) format was proposed [10, 13], which combines the good properties of a canonical [8, 6, 1] and Tucker [15] formats: the number of representation

^sThis work was supported by RFBR grants 09-01-12058, 10-01-00757, 11-01-00549, RFBR/DFG grant 09-01-91332, Russian Federation Gov. contracts No. П1112, П940, 14.740.11.0345 and Priority research program of Dep. Math. RAS No. 3 and 5. Part of this work was done during the stay of the author in Max-Planck Institute for Mathematics in Sciences, Inselstraße 22, 04103 Leipzig, Germany and was supported by Promotionstipendium of Max-Planck Gesellschaft.

parameters does not grow exponentially with the dimension (there is no “*curse of dimensionality*”), and the approximation problem is stable and can be solved by the SVD-based algorithm. Surprisingly, this format can be applied also to data of low dimension using the *virtual levels* [16] / *quantization* of indices [9]. For a vector $x = [x(k)]_{k=0}^{n-1}$ of mode size $n = 2^d$ this is the following one-to-one mapping

$$k \leftrightarrow (k_1, \dots, k_d), \quad k_p = 0, 1, \quad p = 1, \dots, d, \quad k = \overline{k_1 \dots k_d} \stackrel{\text{def}}{=} \sum_{p=1}^d k_p 2^{p-1}, \quad (1)$$

that allows to *reshape* vector into a *tensor* $\mathbf{X} = [x(k_1, \dots, k_d)]$ with d binary indices. The TT format for the latter is called *QTT format* and reads

$$x(k) = x(\overline{k_1 k_2 \dots k_d}) = X_{k_1}^{(1)} X_{k_2}^{(2)} \dots X_{k_d}^{(d)}, \quad (2)$$

where each $X_{j_p}^{(p)}$ is an $r_{p-1} \times r_p$ matrix and *border conditions* $r_0 = r_d = 1$ are introduced to make the right-hand side a scalar for each $k = \overline{k_1 \dots k_d}$.

The values r_p are referred to as *QTT ranks* and affect the storage and complexity in numerical work with vectors in the QTT format. As shown in [10, 12, 13], QTT ranks are equal to the ranks of certain *matricisations*, i.e.

$$r_p = \text{rank } X^{(p)}, \quad X^{(p)} = [x^{(p)}(a, b)], \quad x^{(p)}(\overline{k_1 \dots k_p}, \overline{k_{p+1} \dots k_d}) = x(\overline{k_1 \dots k_d}) = x(k). \quad (3)$$

Since $X^{(p)}$ is a $2^p \times 2^{d-p}$ matrix composed of the elements of x , the rank is bounded by its sizes, $r_p \leq \min(2^p, 2^{d-p})$. In the following we will assume that the “ranks of a vector” are the QTT ranks of the corresponding QTT decomposition.

Definition 1. Vectors with $r_p = 1$ are referred to as *rank-one* vectors, and vectors with $r_p = 2^{\min(p, d-p)}$ as *full-rank* vectors.

Random vector, as well as a random matrix, generally has full ranks. However, many function-related vectors have low ranks ($\exp x$, $\sin x$, $\cos x$, x^p) or have low ε -ranks, i.e. can be accurately approximated by a low-rank vectors (x^α , $e^{-\alpha x^2}$, $\frac{\sin x}{x}$, $\frac{1}{x}$ et al) [9, 5, 11].

For $n = 2^d$, the normalized discrete Fourier transform (DFT) reads

$$y(j) = \frac{1}{2^{d/2}} \sum_{k=0}^{2^d-1} x(k) \omega_d^{jk}, \quad \omega_d = \exp\left(-\frac{2\pi i}{2^d}\right), \quad i^2 = -1, \quad (4)$$

where $F_d = \frac{1}{2^{d/2}} [\omega_d^{jk}]_{j,k=0}^{2^d-1}$ is the unitary Fourier matrix. Recently, the Fourier transform algorithm was proposed for vectors of type (2), maintaining the QTT format during the computation [3]. The complexity of m -dimensional Fourier transform of an $n \times n \times \dots \times n$ array with $n = 2^d$ is $\mathcal{O}(m^2 d^2 r^3)$, which grows logarithmically with n . For large m and n this algorithm is faster than the Fast Fourier transform (FFT) algorithm of $\mathcal{O}(mn^m \log n)$ complexity. However, it is important that r , which is the maximum QTT rank of input, output and all intermediate vectors of the algorithm, remains moderate. It is not easy to describe a class of such vectors explicitly. However, it is instructive to do this in the simplest case of rank-one vectors.

In this paper we describe the class of rank-one vectors with rank-one Fourier images. Also we give an example of rank-one vector that has full-rank Fourier image. This shows that Fourier transform is nontrivial operation that can increase QTT ranks of a vector to the maximum. Finally, by numerical experiments we show that practical ε -ranks of Fourier images of certain rank-one vectors (including the randomly distributed vectors) are moderate even for vectors of very large mode sizes.

2. Rank-one vectors with rank-one Fourier images

Since the QTT ranks do not change with vector scaling, we can consider only normalized vectors (zero vector, a trivial answer, is not interesting). We start from three examples of rank-one vectors that have rank-one Fourier images.

Example 1. A column of $2^d \times 2^d$ identity matrix. A unit vector

$$x = e_{k^*}, \quad \text{i.e. } x(k) = \delta(k - k^*), \quad \text{where } \delta(z) \stackrel{\text{def}}{=} \begin{cases} 1, & z = 0, \\ 0, & z \neq 0, \end{cases}$$

has QTT ranks one, i.e. has the decomposition (2) with all scalar cores,

$$x(k) = \delta(k - k^*) = \delta(\overline{k_1 \dots k_d} - \overline{k_1^* \dots k_d^*}) = \delta(k_1 - k_1^*) \dots \delta(k_d - k_d^*).$$

The Fourier image, $y = F_d x$, is a discretized exponent function with QTT ranks one,

$$y(j) = \frac{1}{2^{d/2}} \exp\left(-\frac{2\pi i}{2^d} k^* j\right) = \frac{1}{2^{d/2}} \exp\left(-\frac{2\pi i}{2^d} k^* j_1\right) \exp\left(-\frac{2\pi i}{2^{d-1}} k^* j_2\right) \dots \exp\left(-\frac{2\pi i}{2} k^* j_d\right).$$

Example 2. Vector $x = \frac{1}{2^{d/2}} \left[\exp\left(\frac{2\pi i}{2^d} j^* k\right) \right]_{k=0}^{2^d-1}$, a discretized exponent with frequency which is an integer multiple of $\frac{2\pi i}{2^d}$, is a rank-one vector with rank-one Fourier image $y = F_d x = e_{j^*}$.

Example 3. For $d = 1$ any vector of size $2^d = 2$ has both QTT ranks one, $r_0 = r_1 = 1$, as well as its Fourier image.

In the following we will show that any rank-one vector with rank-one Fourier image can be represented as a tensor product of the considered examples. Note that the QTT cores of a rank-one vector are unique up to the scaling, i.e. the scaling coefficient can be arbitrary distributed between the QTT cores without changing the result. In the following theorem we describe a class of equivalent rank-one QTT decompositions by one element, and show that a particular QTT representations of the rank-one vector with rank-one Fourier has a specific form.

Theorem 1. A rank-one vector x of size 2^d has rank-one Fourier image, iff the QTT decomposition

$$x(k) = x(\overline{k_1 k_2 \dots k_d}) = x_{k_1}^{(1)} x_{k_2}^{(2)} \dots x_{k_d}^{(d)},$$

after appropriate scaling of QTT cores can be written for some $c = 1, \dots, d$ as follows

$$\begin{aligned} x_{k_p}^{(p)} &= \delta(k_p - k_p^*), \quad k_p^* = 0, 1, \quad \text{for } p < c; \\ x_{k_c}^{(c)} &\text{ is arbitrary;} \\ x_{k_p}^{(p)} &= \frac{1}{\sqrt{2}} \exp\left(\frac{2\pi i}{2^{d-p+1}} j^* k_p\right), \quad \text{for } p > c. \end{aligned} \quad (5)$$

Proof. For $d = 1$ the statement holds, see Example 3. Suppose it holds for any vector of size 2^{d-1} and consider rank-one vector with rank-one Fourier image of size 2^d ,

$$y_{j_1}^{(1)} y_{j_2}^{(2)} \dots y_{j_d}^{(d)} = \frac{1}{2^{d/2}} \sum_{k_1 \dots k_d} x_{k_1}^{(1)} \dots x_{k_{d-1}}^{(d-1)} x_{k_d}^{(d)} \omega_d^{jk}.$$

Write these equations separately for $j_1 = 0$ and $j_1 = 1$,

$$\begin{aligned} y_0^{(1)} y_{j_2}^{(2)} \dots y_{j_d}^{(d)} &= \frac{x_0^{(d)} + x_1^{(d)}}{2^{d/2}} \sum_{k_1 \dots k_{d-1}} x_{k_1}^{(1)} \dots x_{k_{d-1}}^{(d-1)} \omega_{d-1}^{j'k'}, \\ y_1^{(1)} y_{j_2}^{(2)} \dots y_{j_d}^{(d)} &= \frac{x_0^{(d)} - x_1^{(d)}}{2^{d/2}} \sum_{k_1 \dots k_{d-1}} x_{k_1}^{(1)} \dots x_{k_{d-1}}^{(d-1)} \omega_d^{k'} \omega_{d-1}^{j'k'}, \end{aligned} \quad (6)$$

where $k = \overline{k_1 \dots k_d}$, $j' = \overline{j_2 \dots j_d}$, $k' = \overline{k_1 \dots k_{d-1}}$. We come to the radix-2 recurrence relation, that was known to Gauss [4, 7] and lays behind the Cooley-Tukey FFT algorithm [2]. If both $y_0^{(1)} = 0$ and $y_1^{(1)} = 0$ then $y = F_d x = 0$ and since F_d is nonsingular we have $x = 0$, a trivial case. Three non-trivial cases are possible.

First, $y_0^{(1)} \neq 0$ and $y_1^{(1)} = 0$, leads to $x_0^{(d)} = x_1^{(d)}$ and $y' = F_{d-1} x'$, where half-size vectors x' and y' have QTT ranks one,

$$x'(k') = x'(\overline{k_1 \dots k_{d-1}}) = x_{k_1}^{(1)} \dots x_{k_{d-1}}^{(d-1)}, \quad y'(j') = y'(\overline{j_2 \dots j_d}) = y_{j_2}^{(2)} \dots y_{j_d}^{(d)}.$$

Second case, $y_0^{(1)} = 0$ and $y_1^{(1)} \neq 0$, leads to $x_0^{(d)} = -x_1^{(d)}$ and $y' = F_{d-1} \Omega_d x'$, where $\Omega_d = \text{diag}\{\omega_d^{k'}\}_{k'=0}^{2^{d-1}-1}$ and $\Omega_d x'$ has QTT ranks one as well as x' . With proper scaling, we summarize these two cases to

$$y_{j_1}^{(1)} = \delta(j_1 - j_1^*), \quad x_{k_d}^{(d)} = \frac{1}{\sqrt{2}} \exp\left(\frac{2\pi i}{2} j_1^* k_d\right), \quad \text{and} \quad y' = F_{d-1} \Omega_d^{j_1^*} x', \quad (7)$$

where $j_1^* = 0, 1$ and vectors y' and $\Omega_d^{j_1^*} x'$ have size 2^{d-1} and QTT ranks one. By the assumption, cores of vector $\Omega_d^{j_1^*} x'$ are given by (5), which means

$$\begin{aligned} \exp\left(-\frac{2\pi i}{2^{d-p+1}} j_1^* k_p\right) x_{k_p}^{(p)} &= \delta(k_p - k_p^*), \quad k_p^* = 0, 1, \quad \text{for } p = 1, \dots, c-1; \\ \exp\left(-\frac{2\pi i}{2^{d-c+1}} j_1^* k_c\right) x_{k_c}^{(c)} &\text{ is arbitrary;} \\ \exp\left(-\frac{2\pi i}{2^{d-p+1}} j_1^* k_p\right) x_{k_p}^{(p)} &= \frac{1}{\sqrt{2}} \exp\left(\frac{2\pi i}{2^{d-p}} j_1^* k_p\right), \quad \text{for } p = c+1, \dots, d-1. \end{aligned}$$

Moving the scaling coefficients to the core $x^{(c)}$, we result in (5) with $j^* = 2j'_* + j_1^*$.

Finally, consider the case $y_0^{(1)} \neq 0$ and $y_1^{(1)} \neq 0$ in (6). Then

$$y' = \alpha F_{d-1} x' = \beta F_{d-1} \Omega_d x',$$

with above-defined x' and y' and some non-zero scalars α and β , that can be always chosen unit in modulus. Since F_{d-1} is nonsingular, the last equation gives

$$x'(k') = e^{i\varphi} \exp\left(-\frac{2\pi i}{2^d} k'\right) x'(k'), \quad k' = 0, \dots, 2^{d-1} - 1,$$

that holds only for columns of identity $2^{d-1} \times 2^{d-1}$ matrix, $x' = e_{k'_*}$. This vector also has the QTT decomposition of the form (5) with $c = d$, that completes the proof. \square

Directly from the proof of Theorem 1 we colclude the following.

Theorem 2. If a rank-one vector of size 2^d has rank-one Fourier image then all intermediate vectors of the Cooley-Tukey algorithm have QTT ranks one.

3. Rank-one vector with full-rank image

In the Example 2 we show that rank-one vector

$$x(k) = \frac{1}{2^{d/2}} \exp\left(\frac{2\pi i}{2^d} f k\right), \quad k = 0, \dots, 2^d - 1,$$

has rank-one Fourier image for integer $f = j^*$. Now we consider $f \notin \mathbb{Z}$ and prove that Fourier image $y = F_d x$ has full QTT ranks. Using the power series formula, we compute

$$y(j) = \frac{1}{2^d} \sum_{k=0}^{2^d-1} \exp\left(\frac{2\pi i}{2^d} f k\right) \exp\left(-\frac{2\pi i}{2^d} j k\right) = \frac{1}{2^d} \frac{1 - \exp(2\pi i(f-j))}{1 - \exp\left(\frac{2\pi i}{2^d}(f-j)\right)}.$$

Then, using $1 - e^{2i\varphi} = -2ie^{i\varphi} \sin \varphi$, we come to

$$y(j) = \frac{1}{2^d} \frac{\exp(\pi i f) \sin(\pi f)}{\exp\left(\frac{\pi i}{2^d}(f-j)\right) \sin\left(\frac{\pi}{2^d}(f-j)\right)} = \alpha \frac{\exp\left(\frac{2\pi i}{2^d} j\right)}{\sin\left(\frac{\pi}{2^d}(j-f)\right)},$$

where $\alpha = \frac{1}{2^d} \exp(\pi i f (1 - \frac{1}{2^d})) \sin \pi f$. Following (3), QTT ranks of Fourier image y are equal to the ranks of unfoldings,

$$r_p = \text{rank } Y^{(p)}, \quad Y^{(p)} = [y^{(p)}(a, b)], \quad a = \overline{j_1 \dots j_p}, \quad b = \overline{j_{p+1} \dots j_d},$$

$$y^{(p)}(a, b) = y(a + 2^p b) = \alpha \frac{\exp\left(\frac{2\pi i}{2^d} a + \frac{2\pi i}{2^q} b\right)}{\sin\left(\frac{\pi}{2^d}(a-f) + \frac{\pi}{2^q} b\right)},$$

where $p + q = d$. Also, $f = 2^p g + h + \varphi$, where $g \in \mathbb{Z}$, $h = 0, \dots, 2^p - 1$ and $0 < \varphi < 1$. Finally, we represent $\varphi = \varphi_1 + 2^p \varphi_2$ and write

$$\sin\left(\frac{\pi}{2^d}(a-f) + \frac{\pi}{2^q} b\right) = \sin \frac{\pi}{2^d} a' \cos \frac{\pi}{2^q} b' + \cos \frac{\pi}{2^d} a' \sin \frac{\pi}{2^q} b',$$

resulting in $Y^{(p)} = \alpha ACB$, with

$$A = \text{diag} \left\{ \frac{\exp \frac{2\pi i}{2^d} a}{\sin \frac{\pi}{2^d} a'} \right\}, \quad C = \left[\frac{1}{\cot \frac{\pi}{2^d} a' + \cot \frac{\pi}{2^q} b'} \right], \quad B = \text{diag} \left\{ \frac{\exp \frac{2\pi i}{2^q} b}{\sin \frac{\pi}{2^q} b'} \right\}, \quad (8)$$

where $a = 0, \dots, 2^p - 1$, $b = 0, \dots, 2^q - 1$ and $a' = a - h - \varphi_1$, $b' = b - g - \varphi_2$. We can always choose φ_1 and φ_2 such that the denominators in A, B, C are not zero,

$$\begin{aligned} \sin \frac{\pi}{2^d} (a - h - \varphi_1) &\neq 0; \\ \cot \frac{\pi}{2^d} (a - h - \varphi_1) + \cot \frac{\pi}{2^q} (b - g - \varphi_2) &\neq 0; \\ \sin \frac{\pi}{2^q} (b - g - \varphi_2) &\neq 0; \end{aligned} \quad \text{for} \quad \begin{aligned} a &= 0, \dots, 2^p - 1; \\ b &= 0, \dots, 2^q - 1. \end{aligned}$$

With these φ_1 and φ_2 , the diagonal matrices A and B are non-singular since all diagonal elements are non-zero. The rectangular $2^p \times 2^q$ matrix C contains a square submatrix $\left[\frac{1}{s_a + t_b} \right]$ with $a, b = 0, \dots, 2^{\min(p,q)} - 1$, that is also non-singular [14], since it is a Cauchy-Hilbert matrix with distinct s_a and t_b . We conclude that $Y^{(p)}$ has full rank, $r_p = 2^{\min(p,d-p)}$ and therefore vector y has full QTT ranks.

4. Numerical experiments

Numerical computations in scientific computing mostly deal not with exact decompositions, but with approximations and the corresponding ε -ranks, i.e.

$$r_\varepsilon(z) = \min_{\tilde{z}: \|z - \tilde{z}\| \leq \varepsilon \|z\|} r(\tilde{z}). \quad (9)$$

Since the QTT format has d possibly different ranks, it is more convenient to introduce one value $r(\tilde{z})$ to describe the number of parameters that is used to represent \tilde{z} in QTT format. The maximum QTT rank can be used, but sometimes it gives incorrect impression of the “structure complexity”. To account the distribution of all TT ranks r_1, \dots, r_{d-1} , that affect the storage for TT format, we define the *effective* TT rank.

Definition 2.¹ The effective QTT rank r of the TT format with TT ranks r_1, \dots, r_{d-1} and mode sizes n_1, \dots, n_d , is as a positive solution of the quadratic equation

$$\text{mem}(r_1, \dots, r_{d-1}) = \text{mem}(r, \dots, r),$$

where $\text{mem}(r_1, \dots, r_{d-1})$ denotes the amount of memory to store the TT cores,

$$\text{mem}(r_1, \dots, r_{d-1}) = n_1 r_1 + r_1 n_2 r_2 + \dots + r_{d-1} n_d.$$

For the QTT format, all mode sizes are equal 2 and effective QTT rank is defined as

$$r(A) = r, \quad \text{such that} \quad (d-2)r^2 + 2r - \sum_{p=1}^d r_{p-1} r_p = 0. \quad (10)$$

¹This definition was proposed by E. E. Tyrtyshnikov

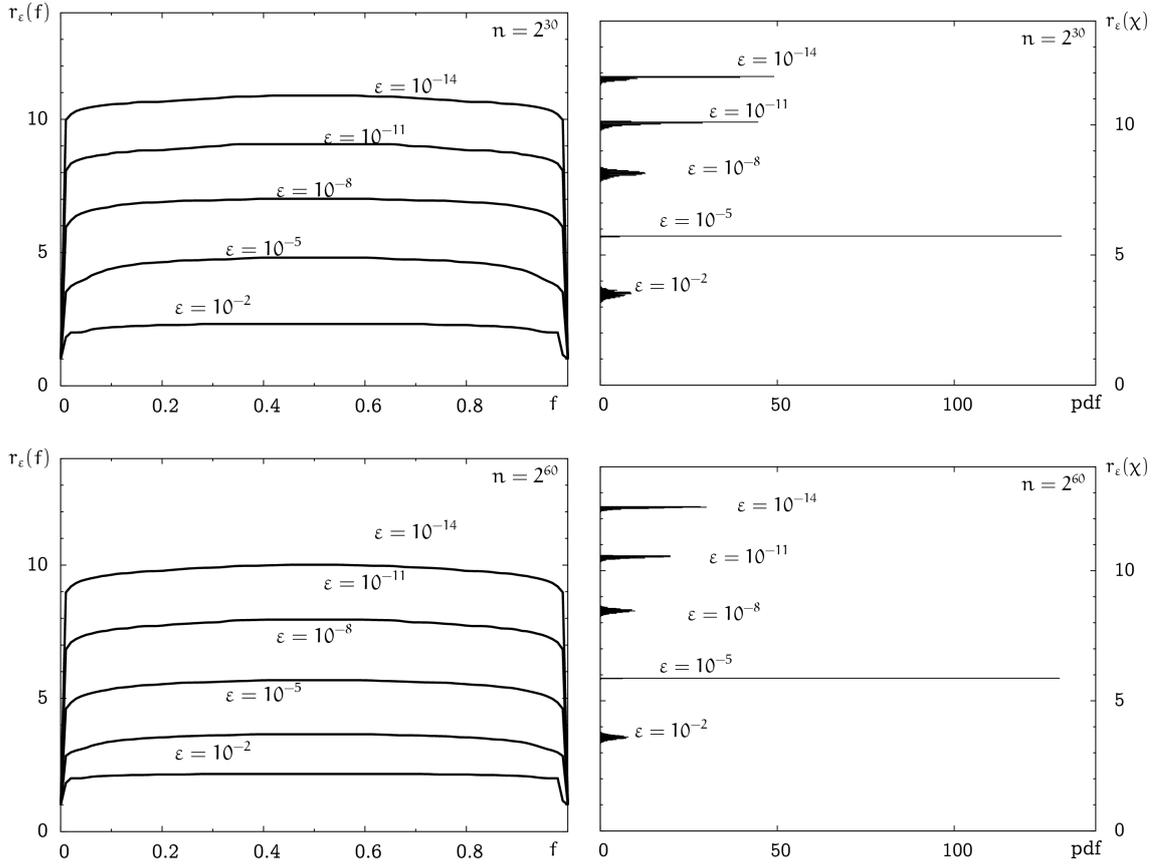


Figure 1. (left) Effective ε -rank of the Fourier image of $\chi = \left[\exp\left(\frac{2\pi i}{2^d} f k\right) \right]_{k=0}^{2^d-1}$, $0 \leq f \leq 1$; (right) effective ε -rank of the Fourier image of random rank-one vector; (top) vectors of size $n = 2^{30}$; (bottom) vectors of size $n = 2^{60}$.

The effective rank is generally a non-integer value. The effective rank of rank-one vector is equal to one. The effective rank of full-rank vector of size 2^d is $r \approx \sqrt{2^d/d}$ and grows exponentially with d , as well as the storage of full array.

On Fig. 1(left) we show the effective ε -rank of the Fourier image of the discretized exponential function $\chi = \left[\exp\left(\frac{2\pi i}{2^d} f k\right) \right]_{k=0}^{2^d-1}$ with frequency $0 \leq f \leq 1$ for different accuracy levels ε . We see that $r_\varepsilon(f)$ tends to one in the small neighbourhoods of zero and one, and almost does not depend on f at certain distance from the sides of the interval. Therefore, we can say that for most of the discretized exponential functions with randomly chosen frequency f the ε -ranks $r_\varepsilon(f)$ depend on ε but not on f . Note also that ε -ranks remain moderate even when the accuracy ε is close to the machine precision, although the exact decomposition is full-rank. The effective ε -rank of the Fourier image even reduces slightly for vectors of very large size $n = 2^{60}$. This shows that even for “bad examples” of data with full-rank images, the approximate Fourier transform using the QTT-FFT algorithm may sufficiently reduce the storage and complexity in comparison with usual FFT.

It is interesting to compare this result with the distribution of ε -ranks of Fourier images of randomly chosen rank-one vectors, see Fig. 1(right). For the QTT vector (2) we set

$x_0^{(p)} = 1$ for $p = 1, \dots, d$ and independently choose real and imaginary parts of $x_1^{(p)}$ from uniform distribution in $[0 : 1]$. We use $5 \cdot 10^8$ samples of vectors of size $n = 2^{30}$ and 10^8 samples² of vectors of size $n = 2^{60}$. It is natural to expect that Fourier images of random vectors would not have a good structure. However, we can see that effective ε -ranks are again quite moderate. Also, the histograms which estimate the probability distribution function of $r_\varepsilon(\chi)$ for rank-one vector χ are very narrow. As in the previous example, we can say that effective ε -ranks actually depend only on accuracy ε and are almost the same for most of the random vectors from the selected set.

Finally, we should note that since the Fourier transform in many dimensions is a tensor product of one-dimensional Fourier transforms, the described results can be directly generalized to multi-dimensional case.

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²The computations were performed using 1024 cores of SKIF-MGU Chebyshev cluster, Moscow State University, Russia

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