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Approximation of Singularities by Quantized-Tensor FEM

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Approximation of Singularities by Quantized-Tensor FEM*

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Abstract

In d dimensions, first-order tensor-product finite-element (FE) approximations of the solutions of second-order elliptic problems are well known to converge algebraically, with rate at most $1/d$ in the energy norm and with respect to the number of degrees of freedom. On the other hand, FE methods of higher regularity may achieve exponential convergence, e.g. global spectral methods for analytic solutions and hp methods for solutions from certain countably normed spaces, which may exhibit singularities.

In this note, we revisit, in one dimension, the tensor-structured approach to the h-FE approximation of singular functions. We outline a proof of the exponential convergence of such approximations represented in the quantized-tensor-train (QTT) format. Compared to special approximation techniques, such as hp, that approach is fully adaptive in the sense that it finds suitable approximation spaces algorithmically. The convergence is measured with respect to the number of parameters used to represent the solution, which is not the dimension of the first-order FE space, but depends only polylogarithmically on that. We demonstrate the convergence numerically for a simple model problem and find the rate to be approximately the same as for hp approximations.

Keywords: Numerical analysis, singular solution, analytic regularity, finite-element method, tensor decomposition, low rank, tensor rank, multilinear algebra, tensor train .
AMS Subject Classification (2000): 15A69, 35C99, 35J25, 65N12, 65N30, 65N35.

1 Tensor train (TT) quantized tensor train (QTT) representations

By *tensors* we mean multidimensional arrays, of which vectors and matrices are examples. The *tensor-train* (*TT* for short) decomposition is a non-linear low-parametric representation of multidimensional arrays, based on the separation of variables and developed in [1, 2]. A l-dimensional $n_1 \times \ldots \times n_l$-vector $\boldsymbol{v}$ is said to be represented in the TT decomposition in terms of two- and three-dimensional arrays $V_1, V_2, \ldots, V_l$, which are called *core tensors*, if

$$\boldsymbol{v}_{i_1,\ldots,i_d} = \sum_{\alpha_1=1}^{r_1} \cdots \sum_{\alpha_{l-1}=1}^{r_{l-1}} V_1(i_1,\, \alpha_1) \cdot V_2(\alpha_1,\, i_2,\, \alpha_2) \cdots V_{l-1}(\alpha_{l-2},\, i_{l-1},\, \alpha_{l-1}) \cdot V_l(\alpha_{l-1},\, i_l) \quad (1)$$

is satisfied for $i_k = 0, \ldots, n_k - 1$ with $k = 1, \ldots, l$. The summation indices $\alpha_1, \ldots, \alpha_{l-1}$ and limits $r_1, \ldots, r_{l-1}$ on the right-hand side of (1) are called, respectively, *rank indices* and *ranks* of the representation. A tensor-train decomposition with l cores, exact or approximate, can be constructed via the low-rank representation of each of $l-1$ matrices; for example, using the SVD. In particular,

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for every $k = 1, \dots, l-1$ the representation (1) implies a rank-r_k factorization of an *unfolding matrix* $\boldsymbol{V}^k$ with the entries $\boldsymbol{V}^k_{\overline{i_1,\dots,i_k},\,\overline{i_{k+1},\dots,i_l}} = \boldsymbol{v}_{i_1,\dots,i_k,i_{k+1},\dots,i_l}$. Here, the overscore denotes the unfolding of a multi-index into a long scalar index: $\overline{i_1,\dots,i_k} = \sum_{\kappa=1}^{k} i_\kappa \prod_{k'=\kappa+1}^{k} n_{k'}$ for the row index, and similarly for the column index, so that $\boldsymbol{V}^k$ is a usual matrix with two "long" indices. The converse statement is also valid: if a vector $\boldsymbol{v}$ is such that the unfolding matrices $\boldsymbol{V}^1, \boldsymbol{V}^2, \dots, \boldsymbol{V}^{l-1}$ are of ranks $r_1, \dots, r_{l-1}$ respectively, then a decomposition with cores $V_1, \dots, V_l$ of corresponding ranks does exist, see [2, theorem 2.1]. Further, the TT format admits efficient approximation and rank-truncation algorithms, which are quasi-optimal with respect to the ℓ^2 norm, see theorem 2.2 with corollaries and algorithms 1 and 2 in [2].

The *quantization* of a dimension of a given tensor consists in folding it into a few modes representing different *levels*, or *scales*, of the former. Consider an n-component vector, where $n = 2^l$ with $l \in \mathbb{N}$, whose components are indexed by i running from 0 to $n-1$. The index can be equivalently represented in the binary form, i.e. by l indices $i_1, \dots, i_l$ taking values in $\{0,1\}$: $(i_1, \dots, i_l) \leftrightarrow i = \overline{i_1, \dots, i_l} = \sum_{q=1}^{l} 2^{l-q}\, i_q$. Here, the overscore denotes such vectorizations of multi-indices, in which the scale of the indices refines from left to right. Thus, i_1 and i_l are the major and minor indices representing the coarsest and finest scales of the vector. The value of i_1 selects between the "left" and "right" halves of $\{0, 1, \dots, 2^l - 1\}$, and the value of i_l, between odd and even elements of the same index set. We refer to the original dimension and index as "physical", in contrast to the "virtual" dimensions and indices produced by quantization. Transformations of this type are quite common: matrices are *unfolded* from representations with linear indexing, arrays are `reshaped` in MATLAB, and the positional notation for numerals relies on a similar bijection.

The idea of applying low-rank tensor decompositions to separate "virtual" dimensions traces back at least to [3], where it appeared in the context of the *canonical polyadic* decomposition of tensors. It has since been widely used with the *tensor-train (TT) decomposition*, which separates indices in a given ordering. Assume that an l-dimensional $2 \times \cdots \times 2$-vector $\boldsymbol{v}$ is obtained from a 2^l-component vector $\boldsymbol{u}$ of one physical dimension, so that $\boldsymbol{v}_{i_1,\dots,i_l} = \boldsymbol{u}_{\overline{i_1,\dots,i_l}}$. Then equation (1) with $n_1 = \ldots = n_l = 2$ provides a *quantized-tensor-train* representation [4, 5, 6] of $\boldsymbol{u}$ with cores $V_1, \dots, V_{l-1}$ and ranks $r_1, \dots, r_{l-1}$. The number of parameters involved in such a representation reads $N_l = 2(r_1 + \sum_{k=2}^{l-1} r_{k-1} r_k + r_{l-1}) \leq 2 l R_l^2$, where $R_l = \max\{r_1, \dots, r_{l-1}\}$.

We note that the *hierarchical tensor representation* [7, 8], a comprehensive exposition of which is given in [9], alone and combined with *tensorization* [10], provide counterparts of the TT and QTT formats respectively. The TT and HT representations have been known in other fields for decades: as *matrix product states (MPS)*, see [11] and references therein, and as the *hierarchical* or *multi-layer MCTDH* method, see [12, 13].

So far, there has been mostly experimental evidence that many applications admit approximations in the TT or related formats with moderate ranks, e.g. $\mathcal{O}(l^\theta)$ with a small $\theta \geq 1$. This property is crucial for the applicability of tensor-structured methods; we refer to the papers [14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24], to the literature survey [25] and more recent works [26, 27, 28].

2 Weighted Sobolev spaces. Analytic regularity of singular functions

In this section, following [29], we recapitulate weighted Sobolev spaces of functions defined in $\Omega = (0,1)$ that may admit singularities at the origin and the corresponding analyticity classes. Analogous constructions in two dimensions are given, for example, in [30, 29, 31].

By $\beta \in [0,1)$ we denote the order of singularities. Assume that $m, \ell \in \mathbb{N} \cup \{0\}$ are such that $m \geq \ell$. For every $k \in \mathbb{N} \cup \{0\}$, we define weight functions $\Phi_{\beta+k}(x) = x^{\beta+k}$ for all $x \in \Omega$, $k \in \mathbb{N} \cup \{0\}$. These weight functions induce weighted Sobolev spaces $\mathrm{H}^{m,\ell}_\beta(\Omega)$: $\mathrm{H}^{m,0}_\beta(\Omega) = \{u :$

$\Omega \to \mathbb{R}:\ \Phi_{\beta+k}\, u^{(k)} \in \mathbb{L}^2(\Omega)$ for $0 \le k \le m\big\}$ and $\mathbb{H}^{m,\ell}_\beta(\Omega) = \big\{u \in \mathbb{H}^{\ell-1}(\Omega):\ \Phi_{\beta+k-\ell}\, u^{(k)} \in \mathbb{L}^2(\Omega)$ for $0 \le k \le m\big\}$ for $\ell \in \mathbb{N}$, where the differentiation is understood in the weak sense. We consider the seminorms $|\cdot|_{\mathbb{H}^{m,\ell}_\beta(\Omega)}$ given by $|u|^2_{\mathbb{H}^{m,\ell}_\beta(\Omega)} = \|\Phi_{\beta+m-\ell}\, u^{(k)}\|^2_{\mathbb{L}^2(\Omega)}$ for all $u \in \mathbb{H}^{m,\ell}_\beta(\Omega)$ and the norms, by $\|u\|^2_{\mathbb{H}^{m,0}_\beta(\Omega)} = \sum_{k=0}^m |u|^2_{\mathbb{H}^{k,0}_\beta(\Omega)}$ for all $u \in \mathbb{H}^{m,0}_\beta(\Omega)$ when $m \in \mathbb{N} \cup \{0\}$ and $\|u\|^2_{\mathbb{H}^{m,\ell}_\beta(\Omega)} = \|u\|^2_{\mathbb{H}^{\ell-1}(\Omega)} + \sum_{k=\ell}^m |u|^2_{\mathbb{H}^{k,\ell}_\beta(\Omega)}$ for all $u \in \mathbb{H}^{m,\ell}_\beta(\Omega)$ when $m, \ell \in \mathbb{N}$ are such that $m \ge \ell$. We note, in particular, that there holds a continuous embedding $\mathbb{H}^{2,2}_\beta(\Omega) \subset \mathbb{C}(\overline{\Omega})$ [29]. We consider the following class of analytic functions.

Definition 2.1. *We say that $u \in \mathfrak{B}^\ell_\beta(\Omega)$ with $\ell \in \mathbb{N} \cup \{0\}$ and $\beta \in [0,1)$ if $u \in \mathbb{H}^{m,\ell}_\beta(\Omega)$ for all integral $m \ge \ell$ and if there exist constants $C_u > 0$ and $\delta_u \ge 1$ such that $|u|_{\mathbb{H}^{m,\ell}_\beta(\Omega)} \le C_u \delta_u^{m-\ell}(m-\ell)!$ for all $m \ge \ell$.*

The functions that belong to $\mathfrak{B}^\ell_\beta(\Omega)$ are analytic in an open domain containing $(0,1]$ with possibly an algebraic singularity at the origin. The embedding $\mathfrak{B}^\ell_\beta(\Omega) \subset \mathbb{H}^{\ell-1}(\Omega)$ follows from the definition for all $\beta \in [0,1)$ and $\ell \in \mathbb{N}$.

For non smooth domains in two dimensions, the standard regularity-shift results for second-order elliptic boundary-value problems, given in terms of standard Sobolev norms, may not hold: the regularity or analyticity of the data does not guarantee that of the solution. However, for the two-dimensional analogues of the spaces $\mathbb{H}^{m,\ell}_\beta(\Omega)$ with $m \ge l \ge 0$ and $\mathfrak{B}^\ell_\beta(\Omega)$ with $\ell \ge 0$, there hold regularity and analyticity shifts, see [30, 29, 31]. The solutions of the aforementioned problems belong to $\mathfrak{B}^2_\beta(\Omega)$ if the data are analytic in the sense of $\mathfrak{B}^\ell_\beta(\Omega)$ with appropriate ℓ.

For such solutions, first-order h-FE approximations constructed on uniform meshes are known to converge only algebraically with respect to the number of mesh nodes. However, the analytic regularity of those solutions may be recovered by hp-approximations, which achieve exponential convergence [29, 31, 32]. In this note we report, using the hp approximation as auxiliary, that the h-FE approximations also achieve exponential convergence when the coefficient vector is represented in the QTT format and with respect to the number of QTT parameters, see N_l in section 1

3 Approximation in h- and hp-spaces

For $l \in \mathbb{N}$, we set $n_l = 2^l$ and $h_l = (n_l+1)^{-1}$. First, we consider a uniform partition $\mathcal{T}_l$ of $\Omega = (0,1)$ with the nodes $t^l_i = i\,h_l$, $i = 0,\dots,n_l+1$, and define the corresponding first-order Courant finite-element space $S^1(\Omega,\mathcal{T}_l)$ as the space of the functions that are linear in each $[t^l_i, t^l_{i+1}]$, $i = 0,\dots,n_l$. Second, we consider a geometrically graded partition $\mathcal{G}_l$ of $\Omega = (0,1)$ with the nodes $x^l_0 = 0$, $x^l_j = 2^{j-1}h_l$, $j = 1,\dots,l$, and $x^l_{l+1} = 1$. For every $j = 1,\dots,l$, we have $x^l_j = t^l_i$ with $i = 2^{j-1}$. For every $p \in \mathbb{N}$, we define the corresponding hp finite-element space $S^p(\Omega,\mathcal{G}_l)$ as the space of the functions that are linear in $[t^l_0, t^l_1]$ and polynomials of degree at most p in each $[x^l_j, t^l_{j+1}]$, $j = 1,\dots,l$.

For every $l \in \mathbb{N}$, we use the spaces $S^p(\Omega,\mathcal{G}_l)$ with $p \sim l$ as auxiliary: we first approximate $u \in \mathfrak{B}^2_\beta(\Omega)$ with an hp-function $v^l \in S^p(\Omega,\mathcal{G}_l)$ and then interpolate v^l by $u^l \in S^1(\Omega,\mathcal{T}_l)$. The benefit of using the hp approximation is that, in fact, it performs low-rank QTT approximation of u: the coefficient of u^l interpolating v^l can be represented in the QTT format *exactly* with ranks bounded by $p+1$.

In [33], the QTT-structured h-FE approximation is shown to converge exponentially with respect to the number of QTT parameters for functions defined on curvilinear polygons and having $\mathfrak{B}^2_\beta$-type singularities at some of the vertices. The basic approach remains the same, as in the one-dimensional setting of the present paper. We outline the key ingredients of the proof below.

First, standard results on the accuracy of hp approximation (see, e.g. [32]) and the analysis of its stability in the $\mathbb{H}^2$-norm yield the following.

Lemma 3.1. *Let* $\beta \in [0,1)$ *and* $u \in \mathfrak{B}^2_\beta(\Omega)$. *Then there exist positive constants* C_1, C_2 *and* b *such that, for every* $l \in \mathbb{N}$, *there exists* $v^l \in S^p(\Omega, \mathcal{G}_l)$ *with* $p = \lceil b\, l \rceil$ *satisfying the interpolation condition* $(u - v^l)(0) = 0 = (u - v^l)(1)$ *and the bounds* $\|u - v^l\|_{\mathbb{H}^1(\Omega)} \leq C_1 2^{-(1-\beta)l}$ *and* $|v^l|_{\mathbb{H}^2(t^l_1,1)} \leq C_2\, l\, 2^{\beta l}$.

Similarly to as in [10, corollary 13], which bounds the QTT ranks of the coefficient of a polynomial in $S^1(\Omega, \mathcal{T}_l)$, one shows the following QTT-rank bound for piecewise-polynomial functions corresponding to partitions $\mathcal{G}_l \subset \mathcal{T}_l$ with $l \in \mathbb{N}$.

Lemma 3.2. *Let* $l, p \in \mathbb{N}$ *and* $v^l \in S^p(\Omega, \mathcal{G}_l)$. *Then the* 2^l*-component vector* $\boldsymbol{v}^l$ *with* $\boldsymbol{v}^l_i = v^l(t^l_i)$, $i = 1, \ldots, 2^l$, *admits a QTT representation with ranks bounded from above by* $p + 2$.

Finally, the nodal reinterpolation of *hp* approximations results in the following.

Theorem 3.3. *Let* $\beta \in [0,1)$ *and* $u \in \mathfrak{B}^2_\beta(\Omega)$. *Then there exist positive constants* C *and* b *such that, for every* $l \in \mathbb{N}$, *there exists* $u^l \in S^1(\Omega, \mathcal{T}_l)$ *satisfying the interpolation condition* $(u - v^l)(0) = 0 = (u - v^l)(1)$ *and the bound* $\|u - u^l\|_{\mathbb{H}^1(\Omega)} \leq C\, 2^{-(1-\beta)l}$ *and such that the* 2^l*-component vector* $\boldsymbol{u}^l$ *with* $\boldsymbol{u}^l_i = u^l(t^l_i)$, $i = 1, \ldots, 2^l$, *admits a QTT representation with ranks bounded from above by* $\lceil b\, l \rceil$.

Theorem 3.3 means that the functions from $\mathfrak{B}^2_\beta(\Omega)$ can be approximated, for every $l \in \mathbb{N}$, by functions from $S^1(\Omega, \mathcal{T}_l)$ determined by N_l parameters with accuracy $\varepsilon \leq C \exp(-c\, N_l^{1/\kappa})$ in the $\mathbb{H}^1$-norm, where $\kappa = 3$ and C and c are positive constants independent of l. Numerically, the same convergence with $\kappa \approx 2$ is achieved, which matches the convergence of *hp* approximations with appropriate $p \in \mathbb{N}$ with respect to $\dim S^p(\Omega, \mathcal{G}_l)$ [32].

4 Numerical experiment

As an illustration, we consider the function $u \in \mathbb{H}^1_0(\Omega)$ given by $u(x) = x^{\alpha + \frac{1}{2}} - x$ for all $x \in \Omega$, with $\alpha = 1/4$, $2/3$ and $3/4$. Our numerical experiments are based on the public-domain TT Toolbox[1] [34].

First, we consider the direct approximation of the nodal interpolant in the QTT format. We define a 2^l-component vector $\boldsymbol{u}^l_{\mathrm{nod}}$ by setting $\boldsymbol{u}^l_{\mathrm{nod}\, i} = u(t^l_i)$ for $i = 1, \ldots, 2^l$ and approximate it in the QTT format with relative accuracy $\varepsilon_l = 2^{-(2-\beta)l}$ in the ℓ^2-norm using the TT Toolbox after quantization: $\boldsymbol{u}^l_{\mathrm{appr}} = \mathtt{tt\_tensor}(\boldsymbol{u}^l_{\mathrm{nod}}, \varepsilon_l)$. This approximation preserves the convergence to u in the $\mathbb{L}^2$- and $\mathbb{H}^1$-norms and reveals the low-rank structure of the nodal interpolants.

Second, we consider a model elliptic second-order boundary-value problem in Ω. For every α, the function u solves the boundary-value problem

$$-u'' + u = f \quad \text{in} \quad \Omega \quad \text{and} \quad u(0) = 0 = u(1) \tag{2}$$

with $f = u - u'' \in \mathbb{H}^{-1}(\Omega)$ given by $f(x) = x^{\alpha + \frac{1}{2}} - x - \left(\alpha^2 - \frac{1}{4}\right) x^{\alpha - \frac{3}{2}}$ for all $x \in \Omega$. For every α, we have $f \notin \mathbb{L}^2(\Omega)$ and both the solution and the right-hand side exhibit singularities at the origin. These singularities may, however, be quantified as follows: $u \in \mathfrak{B}^2_\beta(\Omega)$ and $f \in \mathfrak{B}^0_\beta(\Omega)$ for all real β such that $1 - \alpha < \beta < 1$, i.e. $0 < 1 - \beta < \alpha$. By the Galerkin projection onto $S^1_0(\Omega, \mathcal{T}_l) = S^1(\Omega, \mathcal{T}_l) \cap \mathbb{H}^1_0(\Omega)$, the problem (2) reduces to a linear system $\boldsymbol{A}^l \boldsymbol{u}^l_{\mathrm{sol}} = \boldsymbol{f}^l_{\mathrm{appr}}$ for a 2^l-component vector of coefficients $\boldsymbol{u}^l_{\mathrm{sol}\, i} = u^l_{\mathrm{sol}}(t^l_i)$, $i = 1, \ldots, 2^l$, of the Galerkin solution $u_{\mathrm{sol}} \in S^1_0(\Omega, \mathcal{T}_l)$. Here, $\boldsymbol{f}^l_{\mathrm{appr}}$ is a QTT approximation to the exact load vector assembled by analytical integration, which we obtain with relative accuracy 2^{-l} in the ℓ^2-norm using the TT Toolbox after quantization. That results in $N_l = \mathcal{O}(l^\kappa)$ with $\kappa \approx 2$. The matrix is

[1] We use the master branch of the GitHub version 2.2+ of July 24, 2014 (git tag http://github.com/oseledets/TT-Toolbox/tree/v2.3-4-ge1a3f2c).

Toeplitz tridiagonal and can be represented in the QTT format with ranks bounded by 3, see [35, Lemma 3.1]. We solve the linear system using the AMEn method for the TT-structured solution of linear systems, developed in [36] and available via function `amen_solve2` of the TT Toolbox: $\boldsymbol{u}^l_{\text{sol}} = \texttt{tt\_tensor(amen\_solve2(}\boldsymbol{A}^l\texttt{,}\boldsymbol{f}^l_{\text{appr}}\texttt{,1e-10,...),}\varepsilon_l\texttt{)}$. Here, the solution is truncated with relative accuracy $\varepsilon_l = 2^{-(2-\beta)l}$ in the ℓ^2-norm.

The results are shown in Figures 1–2. Both $\boldsymbol{u}^l_{\text{appr}}$ and $\boldsymbol{u}^l_{\text{sol}}$ achieve $N_l = \mathcal{O}(l^\kappa)$ and the accuracy $\varepsilon_l \leq C \exp(-c\, N_l^{1/\kappa})$ in the $\mathbb{H}^1$-norm, where C and c are positive constants independent of l and $\kappa \approx 2$. That convergence rate is superior to the theoretical estimate with $\kappa = 3$ of Theorem 3.3 and matches the convergence rate of hp approximations in one dimension [32].

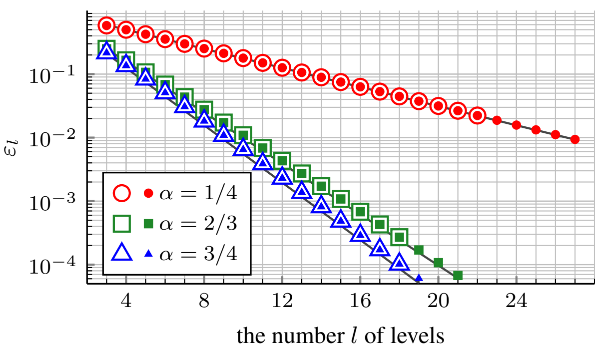

Figure 1: Convergence w.r.t. l. The reference lines correspond to the exponential convergence $\varepsilon_l = 2^{-\alpha l}$.

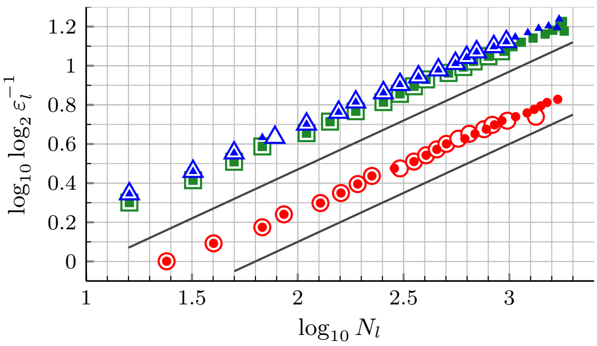

Figure 2: Convergence w.r.t. N_l. The reference lines correspond to the exponential convergence $\log_2 \varepsilon_l = -b\sqrt{N_l}$ with two values of b independent of l.

Figures 1–2. QTT-FEM for $\alpha = \frac{1}{4}$ (red), $\alpha = \frac{2}{3}$ (green) and $\alpha = \frac{3}{4}$ (blue): truncated QTT-FE solutions u^l_{sol} (large empty markers) and QTT-FE approximations u^l_{appr} of the nodal interpolants (small solid markers) of u. Convergence to u with respect to the number l of levels and to the number N_l of QTT parameters. The error is $\varepsilon_l = |\cdot - u|_{\mathbb{H}^1(\Omega)} \,/\, |u|_{\mathbb{H}^1(\Omega)}$.

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