Low rank tensor approximations have been employed successfully, for example, to build surrogate models that can be used to speed up large-scale inference problems in high dimensions. The success of this depends critically on the rank that is necessary to represent or approximate the underlying distribution. In this paper, we develop a-priori rank bounds for approximations in the functional Tensor-Train representation for the case of a Gaussian (normally distributed) model. We show that under suitable conditions on the precision matrix, we can represent the Gaussian density to high accuracy without suffering from an exponential growth of complexity as the dimension increases. Our results provide evidence of the suitability and limitations of low rank tensor methods in a simple but important model case. Numerical experiments confirm that the rank bounds capture the qualitative behavior of the rank structure when varying the parameters of the precision matrix and the accuracy of the approximation.

1 Introduction

Inference problems for high-dimensional random variables appear commonly in scientific computing. In the field of uncertainty quantification, for example, the behavior of a system of interest can be modeled by the pushforward of a random coefficient field by a physical model (often given by a partial differential equation), see e.g. [20], or by the posterior distribution of the corresponding Bayesian inverse problem of estimating parameters based on measured (noisy) data [28]. In typical applications, the underlying stochastic parameter domain is infinite dimensional and has to be discretized (e.g. by a truncated Karhunen-Loève expansion) with tens to thousands of stochastic parameters resulting in a complicated high-dimensional random variable that needs to be investigated. A great deal of effort has been spent on developing numerical methods for such problems. In moderate dimensions, direct polynomial-based approximation methods based on sparse grid approaches [2] can be used to soften the exponential growth of the basis size of the discretized system. However, in general these methods fundamentally cannot escape the curse of dimensionality. Sampling based methods, in particular Monte Carlo or Markov chain Monte Carlo methods, are in principle suitable for inference in very high dimensions [19,20,28]. However, the slow convergence rate and typically long decorrelation times when using Markov chains makes these methods very expensive, in particular when the forward model is complicated and costly to evaluate.

A recently developed methodology to improve the performance of high dimensional inference is to employ a low rank tensor surrogate of the high dimensional function. The surrogate can be used to
represent (or approximate) the function of interest in a parametric format whose complexity only grows polynomially if one assumes bounded ranks. The low rank tensor format can be seen as generalization of the matrix singular value decomposition to higher dimensions. There is no unique way to do this and there is a range of competing formats. Here, we focus on the commonly used Tensor-Train decomposition [23]. For reviews on low rank tensor formats see [13,14,16]. There are many ways one can utilize the low rank parametrization. For example, it can be used in combination with a direct solver (e.g. SGFEM [7,8,18], Bayesian inversion [9]) or to speed up the sampling of the exact distribution [6]. The applicability of this method hinges on the rank that is necessary in order to represent or approximate the underlying high dimensional function. In the applications presented in the papers above, these methods appear to be working well. However, little is known about the theoretical rank behavior in these situations. In some constrained situations, exact rank bounds have been shown [5,12,15,17]. In practice, numerical results show that in many interesting applications high quality approximations can be computed even if the exact representation is not of low rank. Developing theory for this situation appears to be complicated.

In this paper, we present first results on a-priori bounds for the rank of tensor approximations in the case of Gaussian random variables. Due to its ubiquity in statistics as the limiting distribution of (sufficiently regular) averages of random variables, this is a canonical starting point for developing theory of low rank methods. Our consideration is based on locality of correlations between different variables, e.g. bandedness of the covariance matrix, which was also used to reduce the computational complexity of MCMC [21]. When the covariance matrix of the Gaussian is diagonal, the corresponding density reduces to a product of one-dimensional functions which is clearly of rank 1. We show that we can preserve low rank approximability when we are sufficiently close to this setting. We quantify this by looking at the singular spectrum of the subdiagonal blocks of the precision matrix (inverse covariance matrix): we can approximate the densities with low rank if there are only few singular values (Theorem 3.1) or the values are decaying fast (Theorem 3.2). In these cases, we can prove a poly-logarithmic/polynomial growth rate of the ranks in the inverse approximation accuracy $1/\varepsilon$ and in the dimension $d$. However, this result breaks down as we increase the rank of the subdiagonal block matrices or, correspondingly, decrease the decay rate of the singular values.

The paper is organized as follows. In Section 2 we introduce the Tensor-Train format and state all results necessary for the proceeding sections. The main results are presented in Section 3 with their proofs collected in in Section 3.1. In Section 4 we provide numerical examples that confirm the qualitative rates of the ranks stated in Section 3. Finally, we summarize our results in Section 5.

## 2 Low-Rank Tensor Decompositions

In this section, we give a brief overview of the relevant tensor decomposition methods. From an abstract point of view, the goal of these methods is to represent a high dimensional function

$$f : \mathbb{R}^d \to \mathbb{R}$$

as well as its discrete evaluations $T = f(\tilde{Q}) \in \mathbb{R}^{n_1 \times \cdots \times n_d}$ on a tensor grid

$$\tilde{Q} = \times_{i=1}^d \{\xi_1^{(i)}, \ldots, \xi_{n_i}^{(i)}\}$$

with $n_i \in \mathbb{N}$ grid points on each axis. First, we look at the discrete case of the tensor $T$. It is obvious that computing and storing all elements of a tensor $T = f(\tilde{Q})$ directly is prohibitively expensive for anything but very small dimensions. In order to be able to work with $T$, we need an efficient representation whose complexity does not increase exponentially in its dimension. In two dimensions, a low rank representation and optimal approximations are easily computable using the singular value decomposition. There is no clear way to generalize such a decomposition to higher dimensions and there are various formats that manage to transfer some of the properties of the SVD to higher dimensions [13,14]. In this paper, we will use the Tensor-Train (TT) format [23,25] and the corresponding functional Tensor-Train (FTT) format [1] as the low parametric representations. However, the results presented in this paper can be easily generalized to other subspace based tensor formats, e.g. the hierarchical Tucker format [11].

In this section, we briefly define the format and state the properties needed for the following proofs. For an introduction to the format and further details, see [25] and the references in this section.
Definition 2.1 (Discrete Tensor-Train Representation) Let \( r_0, \ldots, r_d \in \mathbb{N} \), and \( T \in \mathbb{R}^{n_1 \times \cdots \times n_d} \) be a \( d \)-dimensional tensor. The tuple of 3-tensors
\[
(G_1, \ldots, G_d) \quad \text{with} \quad G_j \in \mathbb{R}^{r_{j-1} \times n_j \times r_j} \quad \text{where} \quad r_0 = r_d = 1
\]
is called a Tensor-Train (TT) representation of \( T \) if
\[
T(i_1, \ldots, i_d) = G_1(i_1) \cdots G_d(i_d) \quad \text{where} \quad G_j(i_j) := [G_j(l, i, r)]_{l=1}^{r_j-1}.
\]
The tensor \( T \) is represented or approximated by a sequence of three-dimensional tensors \( G_j \) called the TT cores. For \( n \sim n_j \) and bounded ranks \( r \sim r_j \), the number of entries of a TT tensor grows of the order \( O(dnr^2) \). Each entry \( T(i_1, \ldots, i_d) \) is computed by a product of \( d \) matrices which are given by the \( i_j \)-th slice of the 3 dimensional TT core \( G_j(i_j) \) (see Figure 1). In physics literature, this format is also known as the Matrix Product States (MPS) representations of the tensor \( T \). \( \Box \)

\[
\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{cores.png}
\caption{Visualization of the cores of a TT tensor.}
\end{figure}
\]

The Tensor-Train rank structure of \( T \) is determined by the properties of the linear subspaces spanned by the matricizations of the tensor.

Definition 2.2 (Matricization) Let \( T \in \mathbb{R}^{n_1 \times \cdots \times n_d} \) and \( l \in \{1, \ldots, d-1\} \). We call the matrix that results from reshaping \( T \) to
\[
T^{(l)}(i_1, \ldots, i_{l-1}, h+1, \ldots, i_d) \in \mathbb{R}^{n_1 \cdots n_{l-1} \times n_{l+1} \cdots n_d}
\]
the \( l \)-matricization of \( T \).

It is shown in \( [23] \) that the minimal TT ranks needed to exactly represent a tensor in the TT format are given by the matrix ranks of these matricizations.

Theorem 2.3 Let \( T \in \mathbb{R}^{n_1 \times \cdots \times n_d} \). For any TT decomposition \((G_1, \ldots, G_d)\) of \( T \), the \( l \)-th TT rank \( r_l \) fulfills
\[
r_l \geq \operatorname{rank}(T^{(l)})
\]
and there exists a representation that achieves these ranks.

Given the full tensor \( T \), we can compute an optimal TT decomposition by successively computing singular value decompositions. We sketch the procedure: we start with the first matricization
\[
T^{(1)} = U_1 \Sigma_1 V_1^T.
\]
Reshaping the results appropriately, this gives us the first TT core \( G_1 = U_1 \in \mathbb{R}^{r_0 \times n_1 \times r_1} \) as well as the matrix \((\Sigma_1 V_1^T) \in \mathbb{R}^{r_1 n_2 \times n_3 \cdots n_d}\). Again, we compute the SVD
\[
(\Sigma_1 V_1^T) = U_2 \Sigma_2 V_2^T
\]
and set \( G_2 = U_2 \in \mathbb{R}^{r_1 \times n_2 \times r_2} \). This process continues with \((\Sigma_2 V_2^T) \in \mathbb{R}^{r_2 n_3 \times n_4 \cdots n_d}\) and so forth. The resulting cores \((G_1, \ldots, G_d)\) form a TT decomposition of \( T \) with minimal ranks \( [23] \). Since this algorithm relies on subsequent singular value decompositions it is known as TT-SVD.

As an immediate consequence of Theorem 2.3, the exact representation of a random tensor \( T \) in \( \mathbb{R}^{n_1 \times \cdots \times n_d} \) has full rank in each matricization almost surely and its complexity scales exponentially in \( d \). In practice, there is little interest in random tensors. Still, any noise in the entries would make an exact representation impossible even in a case where the underlying tensor is of low rank. It is therefore important to be able to compute approximations and quantify the occurring error. For the Tensor-Train format (and other subspace based formats like the hierarchical Tucker format \( [11] \)) best low rank approximations are guaranteed to exist and the corresponding errors can be easily bounded by again looking at properties of the induced linear subspaces.
Theorem 2.4 Let \( T \in \mathbb{R}^{n_1 \times \cdots \times n_d} \) be a tensor and \( r = (r_0, \ldots, r_d) \) with \( r_0 = r_d = 1 \) be a rank bound. Then, there exists a best approximation \( \tilde{T} \) of \( T \) in the Frobenius norm with TT ranks bounded by \( r \) whose error is bounded by

\[
\|T - \tilde{T}\|_F = \inf_{\text{rank}(G) \leq r} \|T - G\|_F \leq \left( \sum_{i=1}^{d-1} \inf_{\text{rank} A \leq r_i} \|T^{(i)} - A\|_F^2 \right)^{1/2}.
\]

(2.1)

For a proof, see [23]. One of the key features of the TT format is the right-hand side bound in Equation 2.1. This enables us to bound the tensor approximation error by looking at approximations of the matricizations which is a much simpler linear algebra problem. This observation will be the key ingredient that we use to prove the rank bounds in Section 3 In practice, computing exact best approximations is generally intractable, but by subsequently approximating the subspace of each matricization in the TT-SVD algorithm using a truncated singular value decomposition, we can compute an approximation that achieves the bound (2.1). Since the overall approximation error in the TT format is always larger than the error of a single matricization in the Frobenius norm, such an approximation is quasi-optimal with an additional factor of \( \sqrt{d-1} \). The truncated TT-SVD procedure can be implemented efficiently for tensors already given in the TT format [23, Algorithm 1].

To extend this format to a functional setting, we need to find an adequate replacement of the singular value decomposition for analyzing the functional matricizations already given in the TT format [23]. In practice, computing exact best approximations is generally intractable, but by subsequently approximating the subspace of each matricization in the TT-SVD algorithm using a truncated singular value decomposition, we can compute an approximation that achieves the bound (2.1). Since the overall approximation error in the TT format is always larger than the error of a single matricization in the Frobenius norm, such an approximation is quasi-optimal with an additional factor of \( \sqrt{d-1} \). The truncated TT-SVD procedure can be implemented efficiently for tensors already given in the TT format [23, Algorithm 1].

Theorem 2.5 (Schmidt decomposition) Let \( Q_1 \subset \mathbb{R}^l, Q_2 \subset \mathbb{R}^{d-l} \) be open sets and \( Q = Q_1 \times Q_2 \). Let \( \mu = \mu_{Q_1} \otimes \mu_{Q_2} \) be a \( \sigma \)-finite measure and \( f \in L^2(Q) \). Then, there exist complete orthogonal systems

\[
\{\gamma_i\}_{i=1}^\infty \subset L^2_{\mu_{Q_1}}(Q_1), \quad \{\phi_i\}_{i=1}^\infty \subset L^2_{\mu_{Q_2}}(Q_2)
\]

and a non-decreasing sequence \( (\lambda_i)_{i=1}^\infty \subset \mathbb{R} \) such that \( f \) can be expanded as the \( L^2_{\mu}(Q) \) converging series

\[
f = \sum_{i=1}^\infty \sqrt{\lambda_i} \gamma_i \phi_i.
\]

Furthermore, the partial sums \( \sum_{i=1}^k \sqrt{\lambda_i} \gamma_i \phi_i \) are the orthogonal projections of \( f \) and yield the best low rank approximations

\[
\|f - \sum_{i=1}^k \sqrt{\lambda_i} \gamma_i \phi_i\|_{L^2_{\mu}(Q)} = \sqrt{\sum_{i=k+1}^\infty \lambda_i} = \inf_{g \in L^2_{\mu}(Q_1 \times Q_2)} \|f - g\|_{L^2_{\mu}(Q)}.
\]

Similar to the TT-SVD algorithm that computes a decomposition given the full tensor, we can iteratively apply the Schmidt decomposition to the functional matricizations of any function \( f \in L^2(\mathbb{R}^d) \), details of this construction are given in [1]. The result is the following decomposition.

Definition 2.6 Let \( f \in L^2(\mathbb{R}^d) \). We call

\[
f = \sum_{\alpha_1, \ldots, \alpha_d-1}^\infty \gamma_1(\alpha_0, x_1, \alpha_1) \cdots \gamma_d(\alpha_{d-1}, x_d, \alpha_d), \quad (\alpha_0 = \alpha_d = 1), \quad (2.2)
\]

the functional Tensor-Train (FTT) representation of \( f \).

Since we are looking at functional approximations, we can represent \( f \) only by a possibly non-finite series. Similar to the discrete case, we can quantify the error made by cutting the functional Tensor-Train representation to finite ranks \( r \).

Theorem 2.7 Let \( f \in L^2(\mathbb{R}^d) \) and \( r = (r_0, \ldots, r_d) \). Then, there exists an approximation \( \tilde{f} \) of \( f \) with FTT-rank \( r \) whose error is bounded by

\[
\|\tilde{f} - f\|_{L^2(\mathbb{R}^d)} \leq \left( \sum_{i=1}^{d-1} \inf_{g \in L^2(Q_i ' \times Q_i')} \|f - g\|_{L^2(\mathbb{R}^d)}^2 \right)^{1/2}.
\]

(2.3)
This result can be shown by following the steps of \cite{1} Proposition 9 and using Theorem 2.5.

Truncating the representation of \( f \) achieves this bound.

Let \( f \in L^2(\mathbb{R}^d) \cap C(\mathbb{R}^d) \) be a function with FTT rank \( r = (r_0, \ldots, r_d) \). If we compute the evaluation \( f(\hat{Q}) \) of \( f \) on the tensor grid \( \hat{Q} \), it can be written as

\[
 f(\hat{Q})(i_1, \ldots, i_d) = \sum_{\alpha_1, \ldots, \alpha_{d-1}}^r \gamma_1(\xi_{i_1}^{(1)}, \alpha_1) \gamma_2(\alpha_1, \xi_{i_2}^{(2)}, \alpha_2) \cdots \gamma_d(\alpha_{d-1}, \xi_{i_d}^{(d)}).
\]

Therefore, the discrete TT ranks of \( f(\hat{Q}) \) are always bounded by the functional TT ranks of \( f \) independent of the grid it is evaluated on. Of course, the discrete rank might be lower in practice, especially for coarse grids.

2.1 Computing FTT Approximations

For the numerical tests in Section 4 we need to be able to compute approximations of functions in the FTT format. We restrict ourselves to smooth functions \( f : Q \to \mathbb{R} \) on a finite domain

\[
 Q := [-a, a]^d.
\]

We use multivariate polynomial interpolation to approximate \( f \). For simplicity, we will assume the same number of nodes for each dimension. Let \( \hat{Q} := [\xi_1, \ldots, \xi_n]^d \in [-a, a]^n \) be a discrete tensor grid in \( Q \) and \( T := f(\hat{Q}) \). We consider \( T \) as the sample points of a multivariate Lagrange interpolation polynomial

\[
 p_T(x) = \sum_{i_1, \ldots, i_d = 1}^n T(i_1, \ldots, i_d) \prod_{i=1}^d \ell_{i_d}^{(i)}(x_d)
\]

with \( \ell_{i_d}^{(i)} \) the corresponding \( j \)-th one dimensional Lagrange basis functions for the node basis \( \{\xi_1, \ldots, \xi_n\} \). If

\[
 T(i_1, \ldots, i_d) = G_1(i_1) \cdots G_d(i_d)
\]

is a TT tensor of rank \( r = (r_0, \ldots, r_d) \), the FTT rank of the corresponding interpolation polynomial \( p_T \) is bounded by \( r \) since it can be written as

\[
 p_T(x) = \sum_{(\alpha_1, \ldots, \alpha_{d-1})}^r \left( \sum_{i_1=1}^n G_1(i_1, \alpha_1) \ell_{i_1}^{(1)}(x_1) \right) \cdots \left( \sum_{i_d=1}^n G_d(\alpha_{d-1}, i_d) \ell_{i_d}^{(d)}(x_d) \right).
\]

To avoid the instability problems generally associated with polynomial interpolation, we choose the nodes \( \{\xi_1, \ldots, \xi_n\} \) of the Gauss quadrature rule on \([-a, a]\). This choice has the additional benefit that it enables us to approximate integrals of \( f \), and in particular also its \( \ell^2 \) norm, with high accuracy. Since we use the unscaled Lebesgue product measure on \( Q \), the nodes are given by the transformed roots of the \( n \)-th Legendre polynomial. The resulting interpolation polynomial \( p_T \) in (2.4) can be efficiently evaluated at any point \( x \in \mathbb{R}^d \) using Procedure 3 in \cite{1}.

Assume that we are given the exact evaluation tensors \( T_n \) for growing node sizes \( n \). Then, the interpolation polynomial \( p_n := p_{T_n} \) converges fast to the target function \( f \).

\textbf{Theorem 2.8} For any \( \nu \in \mathbb{N} \), there exists a constant \( C = C(\nu) \) such that the Legendre interpolation polynomial \( p_n \) converges with rate \( \nu \) against \( f \)

\[
 \| f - p_n \|_{L^2(Q)} \leq C(\nu)n^{-\nu} |f|_{Q, \nu},
\]

where \( |\cdot|_{Q, \nu} \) denotes the Sobolev semi-norm of the \( \nu \)-th derivative on \( Q \).

For a proof of this theorem, see \cite{1} Proposition 6. To evaluate integrals of \( f \), we apply the corresponding Gaussian quadrature rule. Let \( w = (w_1, \ldots, w_n) \) be the quadrature weights corresponding to the Gauss-Legendre nodes \( \{\xi_1, \ldots, \xi_n\} \). Then, we have

\[
 \int_Q f(x) \, dx \approx \int_Q p_T(x) \, dx = \sum_{i_1, \ldots, i_d = 1}^n (T \circ W)(i_1, \ldots, i_d) \quad \text{with} \quad W := \bigotimes_{i=1}^d w
\]

where

\[
 Q_1 := \mathbb{R}^d \quad \text{and} \quad Q_2 := \mathbb{R}^{d-1}.
\]
where \(\circ\) denotes the Hadamard product of tensors. Using this, we can easily determine the \(L^2\) norm of \(p_T\) by computing the Frobenius norm of the suitably scaled evaluation tensor

\[
\|p_T\|_{L^2(Q)} = \|T \circ \sqrt{W}\|_F.
\]

The Hadamard product and the Frobenius norm are easily computable for tensors in the TT format \cite{Oseledets2011a}.

Using interpolation, we have discretized the problem of computing a functional approximation to computing the tensor \(T\). Of course, the discrete tensor is still far too large to be evaluated directly and we have to employ a structure adapted algorithm for its approximation. Here, we use the TT-cross algorithm described in \cite{Oseledets2011}, namely its rank-adaptive version implemented in the \texttt{rect_cross} class of the \texttt{ttopy} Python package \cite{ttopy}. Using this, we can compute high-accuracy approximations of the discrete evaluation tensors of \(f\).

There are two contributions to the error of \(p_T\): the interpolation error and the error of the TT-cross approximation of the node tensor. For the exact evaluation \(f(\hat{Q})\), the error of the polynomial \(p_f(\hat{Q})\) only depends on the grid \(\hat{Q}\) and, using Theorem \ref{Andre:2012} we can make the relative interpolation error

\[
\delta_{\text{int}} := \|f - p_f(\hat{Q})\|_{L^2(Q)}/\|f\|_{L^2(Q)}
\]

arbitrary small. The approximation of \(T \approx f(\hat{Q})\) introduces an additional error

\[
\delta_{\text{appr}} := \|p_f(\hat{Q}) - p_T\|_{L^2(Q)}/\|f\|_{L^2(Q)} = \|(f(\hat{Q}) - T) \circ \sqrt{W}\|_F/\|f\|_{L^2(Q)}.
\]

The overall error is bounded by

\[
\|f - p_T\|_{L^2(Q)}/\|f\|_{L^2(Q)} \leq \delta_{\text{int}} + \delta_{\text{appr}} =: \delta.
\]

To test the FTT rank structure of \(f\), we compute low rank approximations by truncating the ranks of the TT tensor \(T \circ \sqrt{W}\) to relative accuracy \(\varepsilon\) giving us an approximation \(\tilde{T}\) of \(T\). Consequently, we have

\[
\|p_{\tilde{T}} - f\|_{L^2(Q)} \leq \|p_{\tilde{T}} - p_T\|_{L^2(Q)} + \|p_T - f\|_{L^2(Q)} \leq \|(T - \tilde{T}) \circ \sqrt{W}\|_F + \|p_T - f\|_{L^2(Q)} \leq (\delta + \varepsilon)/\|f\|_{L^2(Q)}.
\]

For \(\varepsilon \gg \delta\), we can ignore the error contribution due to our approximation scheme \(\delta\) and we thus obtain a functional approximation with relative error \(\varepsilon\) and the FTT ranks of \(p_f\).

For a given computed approximation, we need to judge its relative accuracy \(\delta\). The TT-cross procedure generates an error estimate of the completed tensor. To check that we have chosen a sufficiently dense grid, we draw random points on \(Q\) from the target density and compute an importance sampling estimate of the relative interpolation error on \(Q\). If this error agrees with the error estimate of the TT-cross procedure, we accept the completed tensor and use it to investigate the rank structure up to an accuracy \(\varepsilon\) of one order of magnitude less than \(\delta\), see Section \ref{sec:algorithm}.

\section*{3 Bounds on Low Rank Approximability}

In this section, we present our main results. We define two conditions on the precision matrix of a Gaussian density under which we can bound the rank growth for approximations in the functional Tensor-Train format as a function of the dimension and the relative accuracy. The setup is this: given a symmetric positive definite precision matrix \(\Gamma \in \mathbb{R}^{d \times d}\), we consider the density of the Gaussian random variable \(X \sim \mathcal{N}(0, \Gamma^{-1})\)

\[
f_\Gamma : \mathbb{R}^d \to \mathbb{R}, \quad x \mapsto e^{-\frac{1}{2}x^T \Gamma x}
\]

where we have dropped the normalization factor to simplify the notation (this does not influence the ranks). If the precision matrix \(\Gamma = \text{diag}(\gamma_1, \ldots, \gamma_d)\) is diagonal, \(f_\Gamma\) immediately factorizes to

\[
f_\Gamma(x_1, \ldots, x_d) = \prod_{i=1}^d e^{-\frac{1}{2} \gamma_i x_i^2}
\]

which is a rank 1 function. On the other hand, we do not typically see low ranks in approximations when we choose the precision matrix randomly. A reasonable expectation would be that we can approximate the density easily when the precision matrix is “close” to being diagonal.
We relate the approximability of \( f_\Gamma \) to the structure of the subdiagonal blocks of the precision matrix \( \Gamma \). For \( k = 1, \ldots, d - 1 \), we can split \( \Gamma \) into submatrices

\[
\Gamma = \begin{bmatrix}
\Gamma_{1,k} & A_k^T \\
A_k & \Gamma_{2,k}
\end{bmatrix}, \quad A_k \in \mathbb{R}^{(d-k) \times k}.
\]

The subdiagonal block \( A_k \) describes the interaction between the two blocks of variables in the \( k \)-th matricization of \( f_\Gamma \). If \( \Gamma \) is diagonal, we have \( A_k = 0 \) and the blocks do not interact, hence the density factorizes. When \( A_k \neq 0 \), the density does not factorize exactly any more, but if the structure of \( A_k \) is sufficiently simple for each \( k \), we can derive bounds on the ranks necessary to approximate \( f_\Gamma \). We look at two cases: In Theorem 3.1, we assume that each \( A_k \) is a low rank matrix with uniformly bounded singular values and in Theorem 3.2, we assume that the singular spectrum of \( A_k \) decays at an exponential rate. The proofs of both theorems are collected in Section 3.1.

For the first case, we assume that there exists a (small) \( l \in \mathbb{N} \) such that every subdiagonal block \( A_k \) has rank \( A_k \leq l \). We assume further that \( A_k \) has singular values \( \sigma_i^k \), \( i = 1, \ldots, l \), that are uniformly bounded and set

\[
\sigma := \max_{k,i} \sigma_i^k.
\]

**Theorem 3.1** Let \( \Gamma \) be a symmetric positive definite precision matrix with low rank subdiagonal blocks as described above. For every \( \varepsilon > 0 \) there exists an approximation \( \hat{f} \) to the Gaussian density \( f_\Gamma \) with

\[
\| f_\Gamma - \hat{f} \|_{L^2(\mathbb{R}^d)} \leq \varepsilon \| f_\Gamma \|_{L^2(\mathbb{R}^d)}
\]

whose FTT-ranks \( R_k \), \( k = 1, \ldots, d - 1 \), are bounded by

\[
R_k \leq \left( 1 + \frac{7 \sigma}{\lambda_{\min}} \right) \log \left( \frac{\sqrt{8d}}{\varepsilon} \right) + \log \left( \frac{e^{3/2} l}{2} \right)^l
\]

(3.2)

\[
\leq \left( 1 + \frac{7 \sigma}{\lambda_{\min}} \right) \log \left( \frac{7 l}{\varepsilon} \right)^l
\]

(3.3)

where \( \lambda_{\min} \) is the smallest eigenvalue of \( \Gamma \).

In the situation described above, the FTT ranks only grow poly-logarithmically in dimension \( d \) and accuracy \( 1/\varepsilon \). By working with a tensor approximation of the density \( f_\Gamma \), we can therefore avoid the curse of dimensionality. There is however a critical exponential dependence on the number of singular values \( l \) in the subdiagonal blocks.

In statistical applications, the structure of a Gaussian distribution is often more conveniently described by its covariance matrix (i.e. by the inverse of the precision matrix). In this case, Theorem 3.1 is still applicable since the rank of the subdiagonal blocks are the same for \( \Gamma^{-1} \) and \( \Gamma \) [10]. As an important special case, we can apply Theorem 3.1 whenever the covariance or the precision matrix is sparsely populated with entries near to the diagonal (e.g. a band matrix).

The strict low rank requirement can be replaced by a strong decay rate for the singular values. We assume that for all \( k \)-matricizations, the following exponential decay property for the singular values of the corresponding subdiagonal block holds

\[
\sigma_i^k \leq \alpha e^{-\theta i}.
\]

(3.4)

**Theorem 3.2** Let \( \Gamma \) be a symmetric positive definite precision matrix with exponentially decaying singular values in each subdiagonal block as described above. For every \( \varepsilon > 0 \) there exists an approximation \( \hat{f} \) to the Gaussian density \( f_\Gamma \) with

\[
\| f_\Gamma - \hat{f} \|_{L^2(\mathbb{R}^d)} \leq \varepsilon \| f_\Gamma \|_{L^2(\mathbb{R}^d)}
\]

whose FTT-ranks \( R_k \), \( k = 1, \ldots, d - 1 \), are bounded by

\[
R_k \leq \exp \left( \frac{3 \alpha}{\lambda_{\min} \theta} \right) \left( 3 \log \left( \frac{C d}{\varepsilon} \right) \right) \frac{2 \log(C \varepsilon)}{d}
\]

(3.5)

\[
= \exp \left( \frac{3 \alpha}{\lambda_{\min} \theta} \right) \left( \frac{C d}{\varepsilon} \right) \frac{3 \log(3 \log(C d))}{d}
\]

(3.6)
with
\[ C := \max \left\{ \sqrt{8 \frac{5}{\theta}} \frac{e^{\theta}}{1 + e^{\theta} \lambda_{\min}} \right\} \]
where \( \lambda_{\min} \) is the smallest eigenvalue of \( \Gamma \).

Compared to (3.2) from Theorem 3.1, the exponent in (3.5) now has a logarithmic dependence on the dimension \( d \) and accuracy \( 1/\varepsilon \). The reformulation in (3.6) shows that this cannot be neglected: If we ignore the log-log term in the exponent, the equation states a polynomial growth rate of the ranks in the dimension \( d \) and the accuracy \( 1/\varepsilon \) which is substantially worse than the poly-logarithmic rate in Theorem 3.1. This is consistent with our interpretation of the complexity associated with a Gaussian density. Given a certain target accuracy, we can ignore all interactions between the two variable blocks of a matricization described by singular values below a certain threshold since their influence on the density is negligible. As we increase the approximation accuracy, we need to refine our resolution of the dependencies between the blocks of the matricizations, which, according to Theorem 3.1, results in a logarithmic growth of the rank per singular value we look at. However, we also need to decrease the threshold, thereby increasing the number of singular values we need to account for. We will see in Section 3.1 that the number of singular values we have to look at also grows logarithmically in \( 1/\varepsilon \). Combined, this indicates a rate of roughly
\[
\log(1/\varepsilon)^{\log(1/\varepsilon)} = (1/\varepsilon)^{\log \log(1/\varepsilon)}
\]
for \( \varepsilon \ll 1 \) which is similar to the bound in the theorem. Similarly to the dependence on the rank in the previous theorem, this bound depends very sensitively on the decay rate parameters \( \alpha, \theta \) in (3.4).

In both theorems, we have described the FTT ranks by looking at various subdiagonal blocks which describe the correlation between variables of the two dimensions of the matricized function. The structure of these blocks, as well as the ranks necessary for the Tensor-Train approximation, therefore depend on the ordering of the variables. Furthermore, our results can be easily extended to the more general hierarchical Tucker (HT) format [11]. The low rank manifold of HT tensors is, similar to the TT format, described by the ranks of the linear subspaces induced by a generalized notion of matricizations. As with the TT format (Theorem 2.4), approximability in the HT format can be established by approximating the corresponding matricizations. By analyzing the generalized subdiagonal blocks that correspond to the matricizations in the HT format, one can prove equivalent results to Theorem 3.1, 3.2.

### 3.1 Proofs of the Theorems

We have seen in (3.1) that for diagonal precision matrices, the density is of rank 1 since we can write it as product of one dimensional functions. For a general precision matrix, such a multiplicative decomposition would contain additional exponential factors of 2 variables. The general idea behind the proofs of our theorems is to approximate these functions individually with low rank. However, a naive approximation of each function would lead to a rank bound that grows exponentially in the number of off-diagonal terms in \( \Gamma \) which generally grows at least linear in the dimension. In the following, we use the properties of the TT format, in particular Theorem 2.7, as well as suitable coordinate transformations to reduce the number of functions that we need to approximate.

For a general precision matrix, the multiplicative decomposition of the density reads
\[
\rho_{\Gamma}(x) = \prod_{i,j=1}^{d} e^{\frac{1}{2} \Gamma_{i,j} x_i x_j}.
\]
Each of the factors is a two dimensional function of the form
\[
(x, y) \mapsto e^{-\gamma xy} \text{ for some } \gamma.
\]
Interpolating this exponential function with a one dimensional polynomial \( p(t) = \sum_{i=1}^{r} c_i t^{i-1} \in \mathbb{P}_r \) of order \( r \) (and therefore of polynomial rank \( r - 1 \)) yields an approximation
\[
e^{-\gamma xy} \approx p(x, y) = \sum_{i=1}^{r} c_i x^{i-1} \cdot y^{i-1}
\]
which is a sum of \( r \) separated functions and therefore has FTT ranks bounded by \( r \). Before we can apply polynomial interpolation, we need to restrict the function \( f_\Gamma \) to a finite domain. This can be achieved by multiplying with the restriction function

\[
\mathds{1}_\Omega(x) = \begin{cases} 
1, & \text{if } x \in \Omega \\
0, & \text{otherwise}
\end{cases}
\]

which has FTT rank 1 if we restrict to a rectangular domain \( \Omega = I_1 \times \cdots \times I_d \). The overall error is therefore determined by two terms, the error due to the cutoff and the error due to the inexact interpolation, which need to be balanced. We could now apply a cutoff function and approximate each factor of the Gaussian \( f_\Gamma \) with bounded rank, however, the exponential growth in the number of terms would make the resulting bound useless.

Using Theorem 2.7 we only need to prove that we can approximate the individual \( k \)-matricizations

\[
f_\Gamma^k : \mathbb{R}^k \times \mathbb{R}^{d-k} \to \mathbb{R}.
\]

For now, we fix \( k \in \{1, \ldots, d-1\} \). The \( k \)-matricization of any Gaussian density \( f_{\Gamma_t} \) whose precision matrix has the block structure

\[
\Gamma_0 := \begin{bmatrix} \Gamma_1 & 0 \\ 0 & \Gamma_2 \end{bmatrix}, \quad \Gamma_1 \in \mathbb{R}^{k \times k}, \quad \Gamma_2 \in \mathbb{R}^{(d-k) \times (d-k)}
\]

has rank 1 as there is no correlation between the variable blocks \((x_1, \ldots, x_k)\) and \((x_{k+1}, \ldots, x_d)\). This motivates splitting the precision matrix in the diagonal blocks \( \Gamma_1, \Gamma_2 \), and the remaining subdiagonal block \( A \)

\[
\Gamma = \begin{bmatrix} \Gamma_1 & A^T \\ A & \Gamma_2 \end{bmatrix}, \quad A \in \mathbb{R}^{(d-k) \times k}.
\]

At this stage, we would need to approximate an exponential for every non-zero entry in \( A \) which are in general substantially fewer factors than every non-zero off-diagonal entry of \( \Gamma \).

However, we can reduce the number factors further by rotating the coordinate system in for the first \( k \) variables \( \{x_1, \ldots, x_k\} \) and the last \( d-k \) variables \( \{x_{k+1}, \ldots, x_d\} \) respectively. Let \( A = U \Sigma V^T \) be a singular value decomposition of \( A \) and

\[
\tilde{\Gamma} = \begin{bmatrix} V & U \end{bmatrix} \begin{bmatrix} \tilde{\Gamma}_1 & \Sigma^T \\ \Sigma & \tilde{\Gamma}_2 \end{bmatrix} \begin{bmatrix} V^T \\ U^T \end{bmatrix},
\]

where \( \tilde{\Gamma}_1 = V^T \Gamma_1 V \), \( \tilde{\Gamma}_2 = U^T \Gamma_2 U \). We approximate the function \( f_\Gamma \) on the transformed coordinates

\[
\tilde{x}_i = \begin{cases} 
\begin{bmatrix} V \\ U \end{bmatrix}^T x_i & \text{for } i \leq k \\
(V^T[x_{k+1}, \ldots, x_d]^T)_i & \text{otherwise}
\end{cases}
\]

that is, we approximate the function \( f_\Gamma(\tilde{x}) = f_\Gamma(x) \) where

\[
\tilde{\Gamma} := \begin{bmatrix} \tilde{\Gamma}_1 & \Sigma^T \\ \Sigma & \tilde{\Gamma}_2 \end{bmatrix}.
\]

As before, we decompose \( \tilde{\Gamma} \) into

\[
\tilde{\Gamma} = \begin{bmatrix} \tilde{\Gamma}_1 & 0 \\ 0 & \tilde{\Gamma}_2 \end{bmatrix} + \begin{bmatrix} 0 & \Sigma^T \\ \Sigma & 0 \end{bmatrix} =: \tilde{\Gamma}_0 + \tilde{\Gamma}_{\text{SDB}}
\]

and split the transformed density in its rank 1 factor \( f_0 := f_{\tilde{\Gamma}_0} \), and the product of the remaining factors in the subdiagonal block \( f_{\text{SDB}} = f_{\tilde{\Gamma}_{\text{SDB}}} \). The latter factor yields the decomposition

\[
\begin{align*}
{f}_{\text{SDB}}^k(\tilde{x}_1, \ldots, \tilde{x}_k; \tilde{x}_{k+1}, \ldots, \tilde{x}_d) &= e^{-\frac{1}{2} \epsilon^T \tilde{\Gamma}_{\text{SDB}} \epsilon} \\
&= \exp\left(-[\tilde{x}_1, \ldots, \tilde{x}_k]|\Sigma|\tilde{x}_{k+1}, \ldots, \tilde{x}_d]^T\right) \\
&= \prod_{i=1}^{\text{rank } A} \exp\left(-\sigma_i \cdot \tilde{x}_i \cdot \tilde{x}_{k+1}\right) \\
&= : f_1 \cdot f_2 \cdots f_{\text{rank } A}.
\end{align*}
\]

\[3.8\]
where $\sigma_i := \Sigma_{ii}$. It is clear that every low rank approximation of $f_i$ in this matricization

$$f_i(\tilde{x}) \approx \sum_{i=1}^{r} h_i^{(1)}(\tilde{x}_i) h_i^{(2)}(\tilde{x}_{k+1})$$

is also a low rank approximation when retransformed to the original coordinate system. Furthermore, the change of coordinates preserves the $L^2$ norm since the transformation matrix is orthogonal by construction. It is therefore equivalent to show low rank approximability for each matricization in the original and the transformed coordinate system.

To compute the low rank approximation, we restrict to a finite domain in the transformed coordinate system and subsequently approximate each factor $f_i$ by a polynomial. To achieve an overall relative error of $\varepsilon$ for the $k$-th matricization, we allow an error of $\varepsilon/2$ for the subsequent low rank approximation. As a simplification, we restrict $f_\Gamma$ to a square domain $\Omega = [-a,a]^d$ which has to be chosen large enough such that

$$\|f_\Gamma - f_\Gamma|\Omega\|_{L^2(\mathbb{R}^d)} = \|f_\Gamma\|_{L^2(\mathbb{R}^d \setminus \Omega)} \leq \frac{\varepsilon}{2} \|f_\Gamma\|_{L^2(\mathbb{R}^d)} = \frac{\varepsilon}{2} \|f_\Gamma\|_{L^2(\mathbb{R}^d)}.$$ 

This is equivalent to determining a square domain that covers $1 - (\varepsilon/2)^2$ of the volume of the random variable

$$X \sim \mathcal{N}(0, (2\tilde{\Gamma})^{-1}).$$

This can be ensured by choosing $a$ such that every marginal density covers at least $1 - (\varepsilon/2)^2/d$ of the weight. Given $\Gamma$, the minimal decay rate that can occur is bounded from below by the minimal eigenvalue

$$\lambda_{\text{min}}(2\tilde{\Gamma}) = 2\lambda_{\text{min}}(\Gamma).$$

Therefore, it is sufficient to choose a larger than the quantile function of the normal distribution for $\sigma^2 = \frac{1}{2\lambda_{\text{min}}(\Gamma)}$, i.e.

$$a \geq \frac{1}{\sqrt{\lambda_{\text{min}}}} \text{erfc}^{-1} \left( \frac{1}{d} \left( \frac{\varepsilon}{2} \right)^2 \right).$$

For simplicity, we bound the inverse complementary error function as in [4] which yields

$$\frac{1}{\sqrt{\lambda_{\text{min}}}} \text{erfc}^{-1} \left( \frac{1}{d} \left( \frac{\varepsilon}{2} \right)^2 \right) \leq \sqrt{\frac{2}{\lambda_{\text{min}}} \log \left( \frac{\sqrt{2d}}{\varepsilon} \right)} := a.$$

(3.9)

Now, each function $f_i$, treated as a univariate function $x \mapsto e^{-\sigma_i x}$, needs to be approximated by a polynomial on the domain

$$\tilde{\Omega} = [-a^2, a^2].$$

In general, the subblock matrices $A$ could have full rank and, assuming order $O(1)$ interpolations of the factors, the rank of the approximation still increases exponentially in the dimension $d$. This means that without structural assumptions on the precision matrix, we cannot expect our approach to show good FTT approximability. The decomposition (3.8) of $f_{\text{SDE}}$ leads to two natural conditions that result in approximable densities, namely restricting the overall rank (Theorem 3.1) or ensuring a fast enough decay of the singular values (Theorem 3.2).

Let $l := \text{rank } A$ be the rank for the $k$-th matricization. We approximate each function $f_i$ in (3.8) by a polynomial $p_i$. To bound the overall error made by doing this, we single out each error pair

$$f_1 \cdots f_l - p_1 \cdots p_l = \sum_{i=1}^{l} p_1 \cdots p_{i-1} (f_i - p_i) f_{i+1} \cdots f_l$$

to get

$$E := \|f_0 [f_1 \cdots f_l - p_1 \cdots p_l] \|_{L^2(\Omega)} \leq \sum_{i=1}^{l} \|f_i - p_i\|_{L^\infty(\Omega)} \|f_0 p_1 \cdots p_{i-1} f_{i+1} \cdots f_l\|_{L^2(\Omega)}.$$  (3.10)
The $L^\infty$ norm of the polynomial approximation is independent of the dimensionality of the underlying space $\tilde{\Omega}$ and only depends on the approximation quality of the exponential function on the one dimensional domain $\tilde{\Omega}$. For simplicity of notation, we identity $f_i$ with its corresponding one dimensional exponential function 

$$f_i: \tilde{\Omega} \to \mathbb{R}, x \mapsto e^{-\sigma_i x}.$$ 

To derive bounds for the error, we apply classical polynomial interpolation theory.

**Lemma 3.3** Let $x_1, \ldots, x_r$ be the roots of the $(r-1)$-th Chebyshev polynomial transformed to the interval $\tilde{\Omega}$. The error of the order $r$ interpolation polynomial $p_i$ of $f_i$ with nodes $x_1, \ldots, x_r$ is bounded by

$$\max_{\tilde{\Omega}} |f_i - p_i| \leq \frac{1}{r! \cdot 2^{r-1}} \left( \sigma_i a^2 \right)^r e^{\sigma_i a^2},$$

Proof The error of a order $r$ polynomial interpolation on the Chebyshev nodes $x_1, \ldots, x_r$ is bounded by

$$|f_i(x) - p_i(x)| \leq \frac{1}{r! \cdot 2^{r-1}} a^{2r} \max_{x \in \tilde{\Omega}} \left| \frac{\partial^r}{\partial x^r} e^{\sigma_i x} \right| \leq \frac{1}{r! \cdot 2^{r-1}} \left( \sigma_i a^2 \right)^r e^{\sigma_i a^2}$$

(see e.g. [3, Corollary 8.11]). For the second part, we use the Sterling approximation

$$\sqrt{2\pi r} \left( \frac{r}{e} \right)^r \leq r!$$

to estimate the factorial term

$$\frac{1}{r! \cdot 2^{r-1}} \leq \frac{1}{\sqrt{2\pi r} \left( \frac{r}{e} \right)^r} \leq \frac{2}{\sqrt{2\pi}} r^{-r} \left( \frac{e}{2} \right)^r \leq r^{-r} \left( \frac{e}{2} \right)^r.$$ 

To get from (3.11) to an estimate of the relative error, we need to relate the $L^2$ norm of the partial approximation

$$\|f_0 \cdot p_1 \cdots p_{i-1} \cdot f_{i+1} \cdots f_l\|_{L^2(\tilde{\Omega})}$$

(3.12)

to the $L^2$ norm of the density. As a preliminary consideration, we quantify the influence of one factor $f_i$ on the norm of the product.

**Lemma 3.4** Let

$$f^* \in L^2(\Omega)$$

and $i \in \{1, \ldots, l\}$. Then, it holds that

$$\|f^* \|_{L^2(\Omega)} \leq \|f^* f_i\|_{L^2(\Omega)} \exp \left( \sigma_i a^2 \right).$$

Proof By the definition of $f_i$, we get

$$f_i(x) = \exp (-\sigma_i x_i x_{i+k}) \geq \exp (-\sigma_i a^2) > 0.$$ 

Using this, we have

$$\|f^*\|_{L^2(\Omega)} = \|f^* f_i\|_{L^2(\Omega)} \leq \|f^* f_i\|_{L^2(\Omega)} \exp \left( \sigma_i a^2 \right).$$

(3.13)

While this is a crude estimate, the additional exponential term in (3.13) already comes up as part of the corresponding polynomial approximation in Lemma 3.3.

**Lemma 3.5** Let

$$\varepsilon_j^{(r)} := \frac{1}{r! \cdot 2^{r-1}} \left( \sigma_j a^2 \right)^r e^{2\sigma_j a^2}, \quad j = 1, \ldots, l,$$

(3.14)

be the product of the $r_j$-th order polynomial interpolation error bound for $f_i$ on $\tilde{\Omega}$ from Lemma 3.3 and the correction factor from Lemma 3.4. The partial approximation term (3.12) can be estimated by

$$\|f_0 \cdot p_1 \cdots p_{i-1} \cdot f_{i+1} \cdots f_l\|_{L^2(\Omega)} \leq \prod_{j=1}^{i-1} \left( 1 + \varepsilon_j^{(r)} \right) e^{\sigma_i a^2} \|f_0 \cdot f_1 \cdots f_l\|_{L^2(\Omega)}.$$
Proof Let \( f^* \in L^2(\Omega) \) and \( \rho \in \{1, \ldots, i-1\} \). Then
\[
\|f^* p_\rho\|_{L^2(\Omega)} \leq \|f^* f_\rho\|_{L^2(\Omega)} + \|f_\rho\|_{L^\infty(\tilde{\Omega})} \|f^*\|_{L^2(\Omega)} \\
\leq (1 + e^{\rho_\rho} \|f_\rho\|_{L^\infty(\tilde{\Omega})}) \|f^* f_\rho\|_{L^2(\Omega)} \\
\leq (1 + \varepsilon_{\rho}^{c}) \|f^* f_\rho\|_{L^2(\Omega)}.
\]
Note that the multiplicative factor does not depend on \( f^* \). Therefore, we can simply extend this inductively to more than one factor
\[
\|f^* p_1 \cdots p_k\|_{L^2(\Omega)} \leq \|f^* p_1 \cdots p_{k-1} f_k\|_{L^2(\Omega)} + \|f_k\|_{L^\infty(\Omega)} \|f^* p_1 \cdots p_{k-1}\|_{L^2(\Omega)} \\
\leq \prod_{j=1}^{k-1} \left(1 + \varepsilon_j^{(r_j)}\right) \left(\|f^* f_1 \cdots f_{k-1} f_k\|_{L^2(\Omega)} + \|f_k\|_{L^\infty(\Omega)} \|f^* f_1 \cdots f_{k-1}\|_{L^2(\Omega)}\right) \\
\leq \prod_{j=1}^{k} \left(1 + \varepsilon_j^{(r_j)}\right) \|f^* f_1 \cdots f_k\|_{L^2(\Omega)}.
\]
Setting \( f^* = f_0 f_{i+1} \cdots f_i, \ k = i - 1 \), and using Lemma 3.4 to add the missing factor \( f_i \) completes the proof.

The following lemma will be useful later to estimate the required order of the interpolation polynomial.

**Lemma 3.6** Let \( c > 0 \). Then it holds that
\[
\left(\frac{c}{c + r}\right)^{c+r} \leq e^{-c}.
\]

**Proof** We look at the difference of the logarithms of both sides
\[
f(r) := \log \left(\left(\frac{c}{c + r}\right)^{c+r}\right) - \log (e^{-c}) = (c + r)(\log(c) - \log(c + r)) + r.
\]
Note that \( f(0) = 0 \). The derivative of \( f \) satisfies
\[
\frac{d}{dr} f(r) = \log(c) - \log(c + r) \leq 0 \quad \text{for} \quad r \geq 0.
\]
Therefore, \( f(r) \leq 0 \) for \( r \geq 0 \) and the result follows from the monotonicity of the logarithm.

### 3.1.1 Proof of Theorem 3.1

At this stage, we need to start making use of the structure of the precision matrix. We start with the low rank case as described in Theorem 3.1. For this, we assume that for every \( k \)-matricization the subdiagonal blocks \( A_k \) have rank \( \|A_k\| \leq l \) where the singular values \( \sigma_i^k, i = 1, \ldots, l \), are uniformly bounded and set
\[
\sigma := \max_{k,i} \sigma_i^k.
\]

**Proof of Theorem 3.1** Again, we fix a matricization \( k \in \{1, \ldots, d - 1\} \) and look at the function \( f_k(\tilde{x}) \) on the transformed domain as in (3.7). As a first step, we bound the rank necessary to construct a low rank approximation with a relative error bounded by \( \varepsilon_M < 1 \) for this matricization. We fix a finite subdomain \( \Omega = [-a, a]^d \) with \( a \) as in (3.9) such that the relative \( L^2 \) error due to the cutoff is bounded by \( \varepsilon_M / 2 \). Additionally, we need to choose a polynomial order \( r_i \) such that the contribution due to the approximation on \( \Omega \) is bounded by \( \varepsilon_M / 2 \). We choose a uniform interpolation order \( r_i = r \) for all \( f_i, i = 1, \ldots, l \). Let
\[
\varepsilon^{(r)} := \frac{1}{r!} \cdot \frac{1}{2r-1} \left(\sigma a^2\right)^r e^{2\sigma a^2}.
\]
Using Lemma 3.3 and Lemma 3.5, we can bound the error $E$ when using an order $r$ polynomial interpolation by

$$E \leq \sum_{i=1}^{l} \| f_i - p_i \|_{L^\infty(\Omega)} \| f_0 \cdot f_1 \cdots f_i - p_i \|_{L^2(\Omega)}$$

$$\leq \left( 1 + \varepsilon^{(r)} \right)^{l-1} l \varepsilon^{(r)} \| f_0 \cdot f_1 \cdots f_l \|_{L^2(\Omega)}.$$

Therefore, we need to choose $r$ large enough such that

$$\left( 1 + \varepsilon^{(r)} \right)^{l-1} l \varepsilon^{(r)} \leq \frac{\varepsilon M}{2}.$$ (3.15)

For any $r$ that satisfies (3.15), we have $\varepsilon^{(r)} \leq \frac{\varepsilon M}{2l}$. We can utilize this to simplify the left-hand side in (3.15) by using

$$\left( 1 + \varepsilon^{(r)} \right)^{l-1} \leq \exp \left( l \log \left( 1 + \frac{\varepsilon M}{2l} \right) \right) \leq e^{\varepsilon M/2} \leq e^{1/2}.$$

Using Lemma 3.3, it is sufficient to choose $r$ large enough such that we can assure

$$\left( \frac{\sigma a^2}{2r} \right)^r e^{2\sigma a^2} \leq \frac{\varepsilon M}{2l e^{1/2}}$$

which is equivalent to

$$\left( \frac{\sigma a^2}{2r} \right)^r \leq \frac{\varepsilon M}{2l e^{1/2} e^{-2\sigma a^2}}.$$ (3.16)

We compute the necessary interpolation order in two steps: First, we set $r_1 := \frac{\sigma a^2}{e}$ which pushes the left-hand side in (3.16) to 1. Then, we can use Lemma 3.6 to bound the remaining part

$$\left( \frac{r_1}{r_1 + r_2} \right)^{r_1 + r_2} \leq e^{-r_2}$$

and as a result compute the second part $r_2$ as

$$\log \left( \frac{2l e^{1/2}}{e^{2\sigma a^2}} \varepsilon_M \right) \leq 2\sigma a^2 + \log \left( l e^{1/2} \frac{2}{\varepsilon_M} \right)$$

$$=: r_2.$$

Then, choosing $r = r_1 + r_2$ is sufficient to guarantee (3.15). Since we cannot interpolate with non-integer order, we need to choose the next larger integer value. To account for this, we simply add 1 to our bound on $r$. Overall, this gives us

$$r \leq \left( \frac{e}{2} + 2 \right) \sigma a^2 + \log \left( l e^{1/2} \frac{2}{\varepsilon_M} \right) + 1$$

$$= \left( \frac{e}{2} + 2 \right) \sigma a^2 + \log \left( l e^{3/2} \frac{2}{\varepsilon_M} \right).$$

Choosing $a$ as in (3.9) such that additional error that comes from restricting to the finite domain $\Omega$ is bounded by $\varepsilon_M/2$ yields

$$r \leq \left( \frac{e}{2} + 2 \right) \frac{2\sigma}{\lambda_{\text{min}}} \log \left( \frac{2\sqrt{2d}}{\varepsilon_M} \right) + \log \left( l e^{3/2} \frac{2}{\varepsilon_M} \right)$$

(3.17)

$$\leq \left( 1 + 7 \frac{\sigma}{\lambda_{\text{min}}} \right) \log \left( \frac{\sqrt{8d}}{\varepsilon_M} \right) + \log \left( e^{3/2} \frac{1}{2} \right)$$

(3.18)

$$\leq \left( 1 + 7 \frac{\sigma}{\lambda_{\text{min}}} \right) \log \left( 7 \frac{\sqrt{d}}{\varepsilon_M} \right)$$

(3.19)
where we used in the second step that \( d \geq 2 \). We have shown that if we restrict \( f_{T} \) to the domain \( \Omega \) and choose the order of our interpolation larger than \((3.18)\) or \((3.19)\), the overall error of a rank \( R = r^{l} \) approximation on \( \mathbb{R}^{d} \) is bounded by

\[
\| f_{T} - 1_{\Omega} f_{0} p_{1} \cdots p_{l} \|_{L^{2}(\mathbb{R}^{d})} \leq \| f_{T} - f_{\tilde{x}} \|_{L^{2}(\mathbb{R}^{d})} + \| f_{T} - f_{0} p_{1} \cdots p_{l} \|_{L^{2}(\Omega)} \leq \varepsilon_{M} \| f \|_{L^{2}(\mathbb{R}^{d})}.
\]

Since we have seen that proving a low rank bound for \( f_{T}(\tilde{x}) \) on the transformed coordinate system is equivalent to proving a low rank bound for \( f_{T}(x) \), this holds for the rank necessary to approximate the \( k \)-th matricization to a specified accuracy. This rank bound does not depend on \( k \in \{1, \ldots, d-1\} \) and we can apply Theorem 2.7 to bound the error of the FTT approximation \( \tilde{f} \) of the density by

\[
\| f_{T} - \tilde{f} \|_{L^{2}(\mathbb{R}^{d})} \leq \sqrt{d-1}\varepsilon_{M} \| f_{T} \|_{L^{2}(\mathbb{R}^{d})}.
\]

Setting \( \varepsilon_{M} := \frac{\varepsilon}{\sqrt{d}} \) completes the proof.

\[\Box\]

### 3.1.2 Proof of Theorem 3.2

The key of proving low rank approximability is having few, well behaved factors \( f_{i} \) that we can interpolate using polynomials. For Theorem 3.1 we enforced this by assuming a low rank which might be limiting in practice. As an alternative, we look at the case of a rapidly decaying singular spectrum. In Theorem 3.2, we assume that for all \( k \)-matricizations, it holds

\[ \sigma^{k}_{i} \leq \alpha e^{-\theta i}. \]

The idea of the proof is to neglect all singular values that are small enough to not perturb the density too much (effectively approximating the corresponding exponential function by 1). First, we need to determine the number of singular values that we have to look at.

**Lemma 3.7** Let \( k \in \{1, \ldots, d-1\} \) and \( 0 < \varepsilon < 1 \). Under the assumptions made above, the error made by neglecting all terms larger than

\[ l \geq \frac{1}{\theta} \log \left( \frac{e^{\theta} 3\alpha a^{2}}{1 + e^{\theta} \frac{2}{2\varepsilon}} \right) \]

in the decomposition \((3.8)\) of the \( k \)-th matricization of \( f_{T} \) is bounded by

\[ \| f_{T} - f_{0} f_{1} \cdots f_{[l]} \|_{L^{2}(\Omega)} \leq \varepsilon \| f_{T} \|_{L^{2}(\Omega)} \]

**Proof** Using our decomposition of \( f_{T} \), we have

\[ \| f_{T} - f_{0} f_{1} \cdots f_{[l]} \|_{L^{2}(\Omega)} = \| f_{T} (1 - (f_{[l+1]} \cdots f_{\text{rank } A})^{-1}) \|_{L^{2}(\Omega)} \leq \| 1 - (f_{[l+1]} \cdots f_{\text{rank } A})^{-1} \|_{L^{2}(\Omega)} \| f_{T} \|_{L^{2}(\Omega)} \]

We need to choose \( l \) large enough such that

\[ \| 1 - (f_{[l+1]} \cdots f_{\text{rank } A})^{-1} \|_{L^{\infty}(\Omega)} = \| 1 - \sum_{j=l+1}^{\text{rank } A} \alpha e^{-\theta j} \tilde{x}_{j} \tilde{x}_{j} \|_{L^{\infty}(\Omega)} = \sum_{j=l+1}^{\text{rank } A} \alpha e^{-\theta j} \leq 1 \leq \varepsilon \]

Since

\[ e^{x} - 1 \leq \frac{1}{\log(2)} x \leq \frac{3}{2} x \text{ for } 0 < x < \log(2) \]

and \( \varepsilon < 1 \) it is sufficient to choose \( l \) large enough such that

\[ \frac{3}{2} \sum_{j=l+1}^{\text{rank } A} \alpha e^{-\theta j} a^{2} \leq \frac{3}{2} \alpha a^{2} \sum_{j=l+1}^{\infty} e^{-\theta j} \leq \frac{e^{\theta} 3\alpha a^{2}}{1 + e^{\theta} \frac{2}{2\varepsilon}} e^{-\theta l} \leq \varepsilon \]

Solving for \( l \) completes the proof.

\[\Box\]

In particular, the number of factors that we need to deal with explicitly grows logarithmically in the target accuracy in each matricization. We proceed similarly as for the low rank case to approximate these terms.
Proof (of Theorem 3.2) We fix a matricization \( k \in \{1, \ldots, d - 1\} \) and construct a low rank approximation of \( f_\Gamma \) with relative error \( \varepsilon_M \). We choose the domain \( \Omega = [-a, a]^d \) with cutoff error \( \varepsilon_M / 2 \) as in (3.9). Let

\[
\theta := \frac{1}{\theta} \log \left( \frac{e^{\theta} \varepsilon_M}{1 + e^{\theta}} \right),
\]

(3.20)

We ignore all singular values \( \sigma_k \) for \( i > l \). This introduces an error which is controlled using Lemma 3.7

\[
\|f_\Gamma - f_0 f_1 \cdots f_l\|_{L^2(\Omega)} \leq \frac{\varepsilon_M}{4} \|f_\Gamma\|_{L^2(\Omega)}.
\]

It remains to choose ranks for the polynomial interpolation of the \( l \) remaining terms. Let

\[
(\varepsilon_i^{(r_i)} := \frac{1}{r_i!2^{r_i-1}} (\alpha e^{-\theta_i} a^2)^{r_i} e^{2\alpha e^{-\theta_i} a^2}
\]

be the product of the interpolation error and one-term norm correction. Similar to before, we can bound the overall error \( E \) using Lemma 3.5 and thus need to choose the ranks such that

\[
E \leq \sum_{i=1}^{l} \prod_{j=1}^{l} \left( 1 + \varepsilon_j^{(r_j)} \right) e^{\sigma_i a^2} \|f_i - p_i\|_{L^\infty(\Omega)} \|f_\Gamma\|_{L^2(\Omega)}
\]

\[
\leq \prod_{i=1}^{l} \left( 1 + \varepsilon_i^{(r_i)} \right) \sum_{i=1}^{l} \varepsilon_i^{(r_i)} \|f_\Gamma\|_{L^2(\Omega)}
\]

\[
\leq \exp \left( \sum_{i=1}^{l} \varepsilon_i^{(r_i)} \right) \sum_{i=1}^{l} \varepsilon_i^{(r_i)} \|f_\Gamma\|_{L^2(\Omega)} \leq \frac{\varepsilon_M}{4} \|f_\Gamma\|_{L^2(\Omega)}.
\]

(3.22)

We can immediately see that for any sequence of \( \left( \varepsilon_i^{(r_i)} \right)_i \) that satisfies (3.22), it holds

\[
\sum_{i=1}^{l} \varepsilon_i^{(r_i)} \leq \frac{1}{4} \quad \text{and} \quad 4e^{\frac{1}{4}} \leq 6.
\]

Therefore, it is sufficient to choose \( (r_i)_i \) large enough such that

\[
\sum_{i=1}^{l} \varepsilon_i^{(r_i)} \leq \frac{\varepsilon_M}{6}.
\]

In the following, we assume that \( l > 1 \), otherwise, the bound in Theorem 3.2 holds trivially. For simplicity, we assume equidistributed errors

\[
\varepsilon_i^{(r_i)} \leq \frac{\varepsilon_M}{6l} \quad \text{for all} \quad 1 \leq i \leq [l].
\]

We use the bound on \( \varepsilon_i^{(r_i)} \) from Lemma 3.3. For each \( i \), we have to choose the order \( r_i \) big enough such that

\[
\left( \frac{\alpha e^{-\theta_i} a^2}{2r_i} \right)^r e^{2\alpha e^{-\theta_i} a^2} \leq \frac{\varepsilon_M}{6l}.
\]

As before, we compute the order in two parts \( r_i = r_i^{(1)} + r_i^{(2)} \). First, we set

\[
r_i^{(1)} := \frac{e^r}{2} \alpha e^{-\theta_i} a^2.
\]

Again, we use Lemma 3.6 to compute \( r_i^{(2)} \) by ensuring that

\[
e^{-r_i^{(2)}} \leq \frac{\varepsilon_M}{6l} e^{-2\alpha e^{-\theta_i} a^2}
\]

which gives us

\[
r_i^{(2)} := 2\alpha e^{-\theta_i} a^2 + \log \left( \frac{6l}{\varepsilon_M} \right).
\]
Together, we get an upper bound for the necessary integer order on level $i$ by
\[
    r_i \leq \left(2 + \frac{e}{2}\right) a e^{-\theta_i} a^2 + \log \left(\frac{6l}{\varepsilon_M}\right) + 1
\]
\[
    \leq \frac{7\alpha}{\lambda_{\min}} e^{-\theta_i} \log \left(\frac{\sqrt{8d}}{\varepsilon_M}\right) + \log \left(\frac{6}{\varepsilon_M} \log \left(\frac{e^{\theta}}{1 + e^{\theta} \varepsilon_M}\right)\right) + 1.
\]

Using the identity $\log(x) \leq x - 1$, we simplify the second term $A$ further
\[
    A \leq \log \left(\frac{6}{\varepsilon_M} \frac{12\alpha}{1 + e^{\theta} \varepsilon_M \lambda_{\min}}\right) + \log \left(\frac{\sqrt{8d}}{\varepsilon_M}\right)
\]
\[
    = \log \left(\frac{6}{\varepsilon_M} \frac{12\alpha}{1 + e^{\theta} \varepsilon_M \lambda_{\min}}\right) + \log \log \left(\frac{\sqrt{8d}}{\varepsilon_M}\right).
\]

Thus
\[
    r_i \leq \frac{7\alpha}{\lambda_{\min}} e^{-\theta_i} \log \left(\frac{\sqrt{8d}}{\varepsilon_M}\right) + \log \left(\frac{6}{\varepsilon_M} \frac{12\alpha}{1 + e^{\theta} \varepsilon_M \lambda_{\min}}\right) + \log \left(\frac{\sqrt{8d}}{\varepsilon_M}\right)
\]
\[
    \leq \frac{7\alpha}{\lambda_{\min}} e^{-\theta_i} \log \left(\frac{C \sqrt{d}}{\varepsilon_M}\right) + 3 \log \left(\frac{C \sqrt{d}}{\varepsilon_M}\right)
\]
\[
    \leq \left(1 + \frac{3\alpha}{\lambda_{\min}} e^{-\theta_i}\right) 3 \log \left(\frac{C \sqrt{d}}{\varepsilon_M}\right)
\]

with
\[
    C := \max \left\{\sqrt{8}, \frac{5}{\theta}, \frac{e^{\theta}}{1 + e^{\theta} \lambda_{\min}}\right\}
\]

independent of dimension $d$ and accuracy $\varepsilon$ (where we used that $d \geq 2$). Comparing the definition of $l$ in (3.20) with (3.23), we can see that this computation additionally yields
\[
    l \leq \frac{2}{\theta} \log \left(\frac{C \sqrt{d}}{\varepsilon_M}\right).
\]

The overall rank is therefore bounded by
\[
    R \leq \prod_{i=1}^{l} r_i \leq \prod_{i=1}^{l} \left(1 + \frac{3\alpha}{\lambda_{\min}} e^{-\theta_i}\right) 3 \log \left(\frac{C \sqrt{d}}{\varepsilon_M}\right)
\]
\[
    \leq \left(\prod_{i=1}^{\infty} \left(1 + \frac{3\alpha}{\lambda_{\min}} e^{-\theta_i}\right) \right) \left(3 \log \left(\frac{C \sqrt{d}}{\varepsilon_M}\right)\right)^t
\]
\[
    \leq \exp \left(\frac{3\alpha}{\lambda_{\min} \theta}\right) \left(3 \log \left(\frac{C \sqrt{d}}{\varepsilon_M}\right)\right)^\# \log \left(\frac{C \sqrt{d}}{\varepsilon_M}\right)
\]
\[
    = \exp \left(\frac{3\alpha}{\lambda_{\min} \theta}\right) \left(\frac{C \sqrt{d}}{\varepsilon_M}\right)^\# \log \left(\frac{3 \log \left(\frac{C \sqrt{d}}{\varepsilon_M}\right)\right)
\]

where we have used
\[
    \prod_{i=1}^{\infty} \left(1 + \frac{3\alpha}{\lambda_{\min}} e^{-\theta_i}\right) \leq \exp \left(\sum_{i=1}^{\infty} \frac{3\alpha}{\lambda_{\min}} e^{-\theta_i}\right) = \exp \left(\frac{3\alpha}{\lambda_{\min} (e^{\theta} - 1)}\right) \leq \exp \left(\frac{3\alpha}{\lambda_{\min} \theta}\right)
\]
in the last inequality. The rest of the proof follows the same steps as the proof of Theorem 3.1. □
First, we fix a set of parameters for the setting of both theorems and vary the number of dimensions.

### 4.1 Dimension

To create a fair test, we try to avoid any structure in the precision matrices other than the one required in the respective theorems. Our approach is to randomize the precision matrices while fixing the singular spectrum of the subdiagonal blocks to a prescribed sequence. We generate these matrices by the following procedure: we start with $M \in \mathbb{R}^{d \times d}$ with elements randomly chosen between $-1$ and $1$. We symmetrize the matrix $M := MM^\top$ and subsequently update the subdiagonal blocks in $M$ by replacing the singular values in the block with the predefined sequence. We alternate between the different subdiagonal blocks until the singular spectrum has converged. To fix a uniform minimal eigenvalue, we add a suitably scaled identity matrix.

Since we can only approximate the function $f_T$ on the finite domain $Q = [-a, a]^d$, we need to choose an appropriate value for $a$. Ideally, we would want to choose a big enough such that the $L^2$ error introduced by the cutoff is below the approximation accuracy that we are interested in. For accuracies up to $\varepsilon = 10^{-13}$, we would need to choose a large value for $a$ and thus a very high numbers of interpolation nodes $n$. On large parts of this domain, the density is effectively zero which makes the tensor completion challenging. However, in practice the ranks do not appear to depend strongly on the domain size $a$ even at high accuracy, see Figure 2. We therefore choose a fixed value of $a = 7$ for all following tests which results in a typical cutoff error between $3 \times 10^{-5}$ and $1 \times 10^{-6}$, depending on the specific example.

### 4.2 Numerical Examples

In this section, we present numerical tests of the FTT rank bounds from Theorem 3.1 and Theorem 3.2. For a choice of precision matrix, we compute a high accuracy representation of the multivariate Gaussian density as described in Section 2.1 and, subsequently, check the FTT ranks that occur after compressing this representation to various accuracies. Our aim here is to test if we can reproduce the qualitative statements made by our theorems. We focus on the dependence of the FTT ranks on the dimension, the approximation accuracy and rank/the decay rate of the singular values in the subdiagonal blocks.

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### 4.5 Numerical Examples

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Figure 3: FTT ranks of approximations of a Gaussian density with randomized precision matrix at fixed relative accuracy $\varepsilon = 10^{-4}$ for varying number of dimensions $d$. The ranks of the individual completions (translucent) as well as the dimension average (opaque) are shown. On the left, the precision matrices have subdiagonal blocks of rank 2 with singular values $\sigma \equiv 1$. On the right, the singular spectrum decays with rate $e^{-j}$. In both cases, the minimal eigenvalue of the precision matrix is set to $\lambda_{\text{min}} = 0.5$.

to produce a dimension-independent estimate.

For the precision matrices with exponentially decaying singular values in the subdiagonal blocks, a sharp increase of the rank between $d = 5$ and $d = 15$ occurs which does not follow the general trend outlined above. This could potentially be explained by the small row/column length of the subdiagonal blocks in low dimensions. For small $d$ this length could be substantially smaller than $l$ in Lemma 3.7, leading to an initial increase of the number of relevant singular values in the subdiagonal blocks as the dimension increases.

4.2 Low-Rank Subdiagonal Blocks

Now, we fix the dimension and look at the FTT ranks when varying the structure of the subdiagonal blocks and the target accuracy. We start with the case of a fixed rank $l$ in each subdiagonal block of the precision matrix. We fix all singular values to be uniformly $\sigma \equiv 1$, set the dimension to $d = 15$, and set the minimal eigenvalue of the precision matrix to $\lambda_{\text{min}} = 0.5$. We compute the approximation of 10 different realizations of precision matrices for the subdiagonal ranks $l \in \{1, 2, 3, 4\}$. Due to memory constrains, we vary the target accuracy of the TT-cross algorithm depending on the subdiagonal rank. The number of interpolation points $n$ varies between 140 and 270 depending on the target accuracy. In all cases, we make sure that the sampled relative error on $Q$ is below the target accuracy. From Theorem 3.1, we expect a polynomial growth rate in the logarithm of the inverse accuracy. To explore this, we look at a log-log plot of the FTT ranks $r$ and the accuracy $\log(1/\varepsilon)$ (meaning we have a log-log scaled x-axis).

In Figure 4, we present the results of this test. To emphasize the growth behavior for the different parameters, we plot the average of the maximal FTT ranks of the approximations (with individual realizations as translucent lines). We can see that at least for our random set of examples, the averaged curve seems to capture the overall behavior well. While there is variation between different realizations of precision matrices, for large values of $\log(1/\varepsilon)$, the FTT rank trajectory in log-log space seems to only differ by a constant. This indicates that the growth behavior of the FTT ranks is primarily dictated by the ranks in the subdiagonal blocks.

After an initial phase, the FTT rank plot appears to be linear in the log-log plane which indicates that the predicted poly-logarithmic growth rate is qualitatively correct. However, the rates in which the rank grows appears to be less than the rate $\log(1/\varepsilon)^l$ suggested by Theorem 3.1. Nevertheless, when we compare the FTT ranks for a fixed accuracy approximation of $\varepsilon = 10^{-4}$ and vary the rank of the subdiagonal block, we can clearly see that on average, the necessary FTT rank increases exponentially in the number of non-zero singular values. Therefore, our predicted exponential dependence on the number of singular values does not appear to be overly pessimistic.
Figure 4: Ranks of the FTT approximation of a 15 dimensional Gaussian density with low rank subdiagonal blocks. On the left, we show a log-log plot of the maximal FTT ranks given the log-accuracy $\log(1/\varepsilon)$ for different subdiagonal block ranks $l$. On the right, we show the growth of the FTT ranks for a fixed relative accuracy $\varepsilon = 10^{-4}$ when increasing the ranks in the subdiagonal blocks.

Figure 5: Ranks of the FTT approximation of a 30 dimensional Gaussian density with exponentially decaying singular values in the subdiagonal blocks. On the left, we show a log-log plot of the maximal FTT ranks given the accuracy $1/\varepsilon$ for different choices of the decay rate $\theta$ of the singular values in the subdiagonal blocks. On the right, we show the growth of the FTT ranks for a fixed relative accuracy $\varepsilon = 10^{-6}$ when decreasing the decay rate $\theta$.

4.3 Exponentially Decaying Singular Values

As a second test, we follow the setup of Section 4.2 but fix the singular spectrum of each subdiagonal block to follow the sequence

$$\sigma_i = e^{-\theta i}$$

for the $i$-th singular value in each matricization $k$ and vary $\theta \in \{2.5, 2, 1.5, 1\}$. We increase the dimension to $d = 30$ to make sure that we have sufficiently large subdiagonal blocks to not cut off relevant values of the singular spectrum. The number of interpolation nodes $n$ varies between 230 and 310.

The result can be seen in Figure 5. Note that compared to Figure 4, the x-axis now describes $1/\varepsilon$ instead of $\log(1/\varepsilon)$. We can see again that the FTT rank trajectories are to a high degree determined by the prescribed singular spectrum. For $1/\varepsilon$ sufficiently big, the rank growth appears to be polynomial in $1/\varepsilon$. This confirms the polynomial growth rate of FTT ranks predicted in Theorem 3.2. In particular, the ranks grow faster in the accuracy than for precision matrices with low-rank subdiagonal blocks. Overall, as in the previous case, the numerical tests largely agree qualitatively with the predictions made by Theorem 3.2.
5 Conclusions

This present paper introduced rigorous a-priori bounds on the necessary rank to represent Gaussian densities in the functional Tensor-Train format to a specified accuracy. We showed that the necessary FTT rank to approximate a density can be related to the singular spectrum of the subdiagonal blocks of its precision matrix. This proves that, given the circumstances outlined in our theorems, the Tensor-Train format can be used as an efficient surrogate of the high dimensional density that does not suffer from the curse of dimensionality. The two conditions we looked at are precision matrices whose subdiagonal blocks are of low rank or have fast decaying singular values. The $\varepsilon$-rank bounds we prove are not sharp, however as the numerical results in Section 4 show, we managed to capture the dependence on accuracy and rank/decay rate on a qualitative level. The dependence on the number of dimensions appears to be overly pessimistic, but this dependence is in part due to fundamental properties of the Tensor-Train format and it is not clear how this can be avoided.

These results can be immediately generalized by utilizing properties of the (functional) Tensor-Train format. This allows us for example to extend our results to sums and (elementwise) products of Gaussian densities. Therefore, our theory also covers cases like Gaussian mixture models where each element of the mixture fulfills one of our precision matrix conditions. Nevertheless, it would be of further interest to establish rank bounds for more general classes of probability distributions (e.g. distributions of the exponential family).

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References

[1] Daniele Bigoni, Allan P Engsig-Karup, and Youssef M Marzouk. Spectral tensor-train decomposition. SIAM Journal on Scientific Computing, 38(4):A2405–A2439, 2016.
[2] Hans-Joachim Bungartz and Michael Griebel. Sparse grids. Acta Numerica, 13:147–269, 2004.
[3] Richard L Burden and J Douglas Faires. Numerical analysis. Cengage Learning, 9, 2010.
[4] Marco Chiani and Davide Dardari. Improved exponential bounds and approximation for the Q-function with application to average error probability computation. In Global Telecommunications Conference, 2002. GLOBECOM’02. IEEE, volume 2, pages 1399–1402. IEEE, 2002.
[5] S. Dolgov and B. Khoromskij. Two-level QTT-Tucker format for optimized tensor calculus. SIAM J. on Matrix An. Appl., 34(2):593–623, 2013.
[6] Sergey Dolgov, Karim Anaya-Izquierdo, Colin Fox, and Robert Scheichl. Approximation and sampling of multivariate probability distributions in the tensor train decomposition. Statistics and Computing, 2019.
[7] Sergey Dolgov, Boris N Khoromskij, Alexander Litvinenko, and Hermann G Matthies. Polynomial chaos expansion of random coefficients and the solution of stochastic partial differential equations in the tensor train format. SIAM/ASA Journal on Uncertainty Quantification, 3(1):1109–1135, 2015.
[8] Sergey Dolgov and Robert Scheichl. A hybrid alternating least squares–TT-cross algorithm for parametric PDEs. SIAM/ASA Journal on Uncertainty Quantification, 7(1):260–291, 2019.
[9] Martin Eigel, Max Pfeffer, and Reinhold Schneider. Adaptive stochastic Galerkin FEM with hierarchical tensor representations. Numerische Mathematik, 136(3):765–803, 2017.
[10] Miroslav Fiedler. Structure ranks of matrices. Linear Algebra and its Applications, 179:119–127, 1993.
[11] Lars Grasedyck. Hierarchical singular value decomposition of tensors. *SIAM Journal on Matrix Analysis and Applications*, 31(4):2029–2054, 2010.

[12] Lars Grasedyck. Polynomial approximation in hierarchical Tucker format by vector-tensorization. Technical report, Institut für Geometrie und Praktische Mathematik, RWTH Aachen, 2010.

[13] Lars Grasedyck, Daniel Kressner, and Christine Tobler. A literature survey of low-rank tensor approximation techniques. *GAMM-Mitteilungen*, 36(1):53–78, 2013.

[14] Wolfgang Hackbusch. *Tensor spaces and numerical tensor calculus*, volume 42. Springer Science & Business Media, 2012.

[15] V. Kazeev, O. Reichmann, and Ch. Schwab. Low-rank tensor structure of linear diffusion operators in the TT and QTT formats. *Linear Algebra and its Applications*, 438(11):4204–4221, 2013.

[16] Boris N Khoromskij. Tensor numerical methods for multidimensional PDEs: theoretical analysis and initial applications. *ESAIM: Proceedings and Surveys*, 48:1–28, 2015.

[17] Boris N Khoromskij and Ivan V Oseledets. DMRG+QTT approach to computation of the ground state for the molecular Schrödinger operator. Technical Report 69, MPI MIS Leipzig, 2010.

[18] Boris N Khoromskij and Christoph Schwab. Tensor-structured Galerkin approximation of parametric and stochastic elliptic PDEs. *SIAM Journal on Scientific Computing*, 33(1):364–385, 2011.

[19] Jun S. Liu. *Monte Carlo Strategies in Scientific Computing*. Springer-Verlag, New York, 2004.

[20] Gabriel J. Lord, Catherine E. Powell, and Tony Shardlow. *An Introduction to Computational Stochastic PDEs*. Cambridge University Press, Cambridge, 2014.

[21] Matthias Morzfeld, Xin T Tong, and Youssef M Marzouk. Localization for MCMC: sampling high-dimensional posterior distributions with local structure. *Journal of Computational Physics*, 380:1–28, 2019.

[22] Ivan Oseledets and Eugene Tyrtyshnikov. TT-cross approximation for multidimensional arrays. *Linear Algebra and its Applications*, 432(1):70–88, 2010.

[23] Ivan V Oseledets. Tensor-train decomposition. *SIAM Journal on Scientific Computing*, 33(5):2295–2317, 2011.

[24] Ivan V Oseledets et al. ttpy - a Python implementation of the TT-toolbox. [https://github.com/oseledets/ttpy](https://github.com/oseledets/ttpy), 2018.

[25] Ivan V Oseledets and Eugene E Tyrtyshnikov. Breaking the curse of dimensionality, or how to use SVD in many dimensions. *SIAM Journal on Scientific Computing*, 31(5):3744–3759, 2009.

[26] Ulrich Schollwöck. The density-matrix renormalization group. *Reviews of modern physics*, 77(1):259, 2005.

[27] Jaromír Šimša. The best $L^2$-approximation by finite sums of functions with separable variables. *Aequationes mathematicae*, 43(2-3):248–263, 1992.

[28] Andrew M Stuart. Inverse problems: a Bayesian perspective. *Acta Numerica*, 19:451–559, 2010.