Computing f-Divergences and Distances of High-Dimensional Probability Density Functions — Low-Rank Tensor Approximations —

Alexander Litvinenko* a, Youssef Marzouk b, Hermann G. Matthies c, Marco Scavino d, and Alessio Spantini b

aRheinisch-Westfälische Technische Hochschule (RWTH) Aachen, Germany
bMIT, Cambridge (MA), USA
cTechnische Universität Braunschweig, Brunswick, Germany
dUniversidad de la República, Instituto de Estadística (IESTA), Montevideo, Uruguay

Abstract

Very often, in the course of uncertainty quantification tasks or data analysis, one has to deal with high-dimensional random variables. Here the interest is mainly to compute characterisations like the entropy, the Kullback-Leibler divergence, more general f-divergences, or other such characteristics based on the probability density. The density is often not available directly, and it is a computational challenge to just represent it in a numerically feasible fashion in case the dimension is even moderately large. It is an even stronger numerical challenge to then actually compute said characteristics in the high-dimensional case. In this regard it is proposed to approximate the discretised density in a compressed form, in particular by a low-rank tensor. This can alternatively be obtained from the corresponding probability characteristic function, or more general representations of the underlying random variable. The mentioned characterisations need point-wise functions like the logarithm. This normally rather trivial task becomes computationally difficult when the density is approximated in a compressed resp. low-rank tensor format, as the point values are not directly accessible. The computations become possible by considering the compressed data as an element of an associative, commutative algebra with an inner product, and using matrix algorithms to accomplish the mentioned tasks. The representation as a low-rank element of a high order tensor space allows to reduce the computational complexity and storage cost from exponential in the dimension to almost linear.

Keywords: high-dimensional probability density, Kullback-Leibler divergence, f-divergence, distance, tensor representation, computational algorithms, low-rank approximation

MSC Classification: 41A05 · 41A45 · 41A63 · 60-08 · 60E07 · 60E10 · 62-08 · 62E17 · 62H10 · 65C20 · 65F55 · 65F60 · 94A17

*Corresponding author: RWTH Aachen, 52072 Aachen, Germany, e-mail: Litvinenko@uq.rwth-aachen.de
1 Introduction

In statistics and probability, and in particular in the vigorous field of uncertainty quantification (UQ) \([44, 88, 87]\), one often has to deal with high-dimensional random variables (RVs) with values in \(\mathbb{R}^d\). Frequently, one is interested in characteristic quantities of interest (QoI), examples are the differential entropy, the Kullback-Leibler or more general \(f\)-divergences, or other such characteristics based on integrals of some function of the probability density function (pdf). Computing such integrals, or just storing a discretised form of the pdf, may become a daunting task for even moderately high dimensions \(d\).

1.1 Motivation and main idea

One apparently quite efficient way to deal with such high-dimensional RVs is to view them as elements of some tensor product space of tensors of high order — typically the order corresponds to the dimension \(d\) \([55]\). Such tensors can be approximated by low-rank tensors, and thus it becomes feasible to deal with them numerically. Here we concentrate solely on real valued continuous RVs which possess a pdf, so another possibility is the representation of the pdf in some computationally advantageous form.

Possible QoIs are often defined or only accessible in some specific representation of the RV. We are thinking of QoIs such as the entropy, the Kullback-Leibler (KL) divergence, or more generally \(f\)-divergences, as well as Hellinger distances, and (central) and generalised moments, to name a few such QoIs \([82, 90, 112]\). Some are defined and can efficiently be computed with a functional representation of the RV, and some are defined and efficiently computed if one has access to the point values of the pdf, the case to be considered here.

The algorithms we formulate are for a compressed discrete representation of the pdf, and we actually use for our computations a low-rank tensor approximation. We sketch three possibilities how to arrive at such a low-rank representation of the density. One is via tensor function representations \([13, 8, 55, 48, 15]\) of the pdf \([30, 103]\), another via an analogous representation of the probabilistic characteristic function (pcf) \([110, 106, 120]\), and a third one is via a low-rank representation of the RV itself — e.g. \([23, 24]\).

Connecting and connected with these different representations — next to the already mentioned pcf—are other well known characterising objects like the moment generating function or the second characteristic or cumulant generating function, and we show how these may be efficiently computed as well in a low-rank tensor format. Motivating factors for an accuracy controlled low-rank tensor compression include the following \([78, 55]\):

- reduce the storage cost to linear or even sub-linear in the dimension \(d\);
- perform algebraic operations in cost linear or even sub-linear in the dimension \(d\);
- combining it with the fast Fourier transform (FFT) yields a superfast FT \([92, 27]\).

On the other hand, general limitations of such a tensor compression technique are that

- it could be time-consuming to compute a low-rank tensor decomposition;
- with sampling or point evaluation, it requires an axes-parallel mesh;
- after algebraic manipulations, a re-compression may be necessary;

It is a fact that there are situations where storage of all items is not feasible, or operating on all items is out of the question, so that some kind of compression has to be employed, and low-rank tensor techniques offer a very promising avenue \([78, 55]\). But for the algorithms shown later in Section 5 all that is required is that the compressed data can be considered as an element of an associative, commutative algebra with an inner product.

Further, the actual computational representation is allowed to be a lossy compression, and the algebraic operations may be performed in an approximate fashion, so as to maintain
a high compression level. We address explicitly the representation of data as a tensor with compression in the form of a low-rank representation. The suggested technique, in order to be employed efficiently, assumes that all involved tensors have a low rank, and the rank is not increasing strongly after linear algebra operations. In Section 6 we show some exemplary numerical examples of applications of this framework to approximate high-dimensional pdfs of α-stable type—which are given only through their pcf—and compute divergences and distances between such probability distributions.

Let us give an example which motivates much of the following formulation and development. Assume that one is dealing with a random vector $\mathbf{ξ}$ in a high-dimensional vector space $\mathbb{R}^d$, i.e. $\mathbf{ξ} = (ξ_1, ..., ξ_d)^T : \Omega \rightarrow \mathbb{R}^d$, defined on a suitable probability space $\Omega$. Further assume that this random vector has a pdf $p_ξ : \mathbb{R}^d \rightarrow \mathbb{R}$, and that we want to compute—as a simple example of the possible tasks envisioned—the differential entropy (see also Eq. (37)), the expectation of the negative logarithm of the pdf. This requires the point-wise logarithm of $p_ξ$:

$$h(p_ξ) := \mathbb{E}(-\ln(p_ξ(y))) := \int_{\mathbb{R}^d} -\ln(p_ξ(y)) p_ξ(y) \, dy.$$ (1)

Even if one has an analytical expression resp. approximation for the pdf $p_ξ$, it still may not be possible to compute the above integral analytically, and so we propose to do this numerically. This immediately provokes the curse of dimensionality, as the numerical evaluation of such high dimensional integrals can be very expensive, with work proportional $n^d$, where $n \in \mathbb{N}$ is a discretisation parameter. In the following, we shall propose one possible approach to alleviate the computational burden.

The goal is a discrete low-rank tensor point evaluation of the pdf. The first starting point is the assumption that one has or may obtain a low-rank tensor function representation [13, 8, 55, 48, 15] of the pdf [30, 103]. The second possible starting point is that one has such a low-rank tensor function of the pcf [86, 110, 106, 120, 10]. Then via the Fourier transform one may come back to the pdf. And the third possibility sketched is that one has a sparse or low-rank representation of a high-dimensional RV. From this one may evaluate the pcf on a tensor grid, and from there then via the Fourier transform again arrive at a low-rank approximation of the pdf.

Further assume that the pdf of the high-dimensional RV has its support in a compact hyper-rectangle, supp $p_ξ := \text{cl}\{y \in \mathbb{R}^d \mid p_ξ(y) \neq 0\} \subseteq \bigtimes_{\nu=1}^d [ξ_\nu^{(\text{min})}, ξ_\nu^{(\text{max})}] \subset \mathbb{R}^d$. A fully discrete representation of the pdf can be achieved (further details will be provided in Section 2) by picking in each dimension $1 \leq \nu \leq d$ an equidistant grid vector $\hat{x}_\nu := (\hat{x}_{1,\nu}, ..., \hat{x}_{M_\nu,\nu})$ of size $M_\nu$, such that for all $\nu$ it holds that $\hat{x}_{i_\nu,\nu} \in [ξ_\nu^{(\text{min})}, ξ_\nu^{(\text{max})}]$ for $1 \leq i_\nu \leq M_\nu$. The size $M_\nu$ could be different for each dimension $\nu$, but for the sake of simplicity here we shall often assume them all equal to $n$, i.e. each $\hat{x}_\nu \in \mathbb{R}^n$. The whole grid will be denoted by $\hat{X} = \bigtimes_{\nu=1}^d \hat{x}_\nu = (\hat{X})_{(i_1, ..., i_d)}$ with $1 \leq i_\nu \leq M_\nu$.

The notation $P := p_ξ(\hat{X})$ will denote the tensor $P \in \bigotimes_{\nu=1}^d \mathbb{R}^{M_\nu} =: T = (\mathbb{R}^n)^d = \mathbb{R}^N$, with dim $T = \prod_{\nu=1}^d M_\nu =: N = n^d$, the components of which are the evaluation of the pdf $p_ξ$ on the grid $\hat{X}$

$$P := p_ξ(\hat{X}) := (P_{i_1, ..., i_d}) := (p_ξ(\hat{x}_{i_1,1}, ..., \hat{x}_{i_d,d})), \quad 1 \leq i_\nu \leq M_\nu, 1 \leq \nu \leq d.$$ (2)

If $n$ and especially the dimension $d$ are even moderately large, the total dimension $N = n^d$ is very quickly a huge number, maybe even so that it is not possible to reasonably store that amount of information.

Sometimes the density $p_ξ$ is—at least approximately—given as an analytical expression, and it may be possible to approximate it [59] through a low-rank function tensor represent-
where each \( p_{\ell,\nu} \) is only a function of the real variable \( y_\nu \) in dimension \( \nu \). This so-called canonical polyadic (CP) tensor representation [59] (cf. Section 4) becomes computationally viable when the rank \( R \) can be chosen fairly small. The multi-dimensional Gaussian distribution with diagonal covariance matrix is an obvious simple case in point with \( R = 1 \). The \( p_{\ell,\nu} \) are evaluated on the grid vector \( \hat{x}_\nu \) for all \( \nu \) and \( \ell \), giving \( p_{\ell,\nu} := (p_{\ell,\nu}(\hat{x}_{1,\nu}), \ldots, p_{\ell,\nu}(\hat{x}_{M,\nu})) \in \mathbb{R}^{M_\nu} \). This is a building block for a possible low-rank CP representation of the tensor \( P \), as now

\[
P \approx \sum_{\ell=1}^{R} \bigotimes_{\nu=1}^{d} p_{\ell,\nu}.
\]

More details and descriptions about this and other low-rank tensor approximations will be given in Section 4. To evaluate now numerically an expression like the differential entropy Eq. (1), the integral is replaced by a numerical quadrature

\[
h(p_\xi) \approx \sum_{i_1=1}^{M_1} \cdots \sum_{i_d=1}^{M_d} - \ln(P_{i_1,\ldots,i_d}) P_{i_1,\ldots,i_d} w_{i_1,\ldots,i_d},
\]

where \( w_{i_1,\ldots,i_d} \) are integration weights, which will all be chosen equal \( w_{i_1,\ldots,i_d} \propto N^{-1} \), cf. Section 2 and Section 3.

The challenge in Eq. (5) is the huge number of terms in the sum. Here the low-rank representation Eq. (4) can be used to advantage, cf. Section 2, but then the challenge is to compute the logarithm in Eq. (5) when \( P \) is in the representation Eq. (4). For this certain algebraic properties of the space \( \mathcal{T} \) will be used, as will be explained in Section 2 and Section 5. There are of course other ways to arrive at a discrete low-rank representation of a high-dimensional function. One group of such possible methods are the various “cross”-procedures [36, 99, 8, 7, 26, 31]. In any case, this is not supposed to be an exhaustive survey of such methods, and only intended to give some hints and point to some possibilities.

At other times the pdf may not be available, but instead the probabilistic characteristic function (pcf) \( \varphi_\xi \) of the pdf

\[
\varphi_\xi(t) := \mathbb{E}(\exp(i \langle \xi \mid t \rangle)) := \int_{\mathbb{R}^d} p_\xi(y) \exp(i \langle y \mid t \rangle) \, dy =: \mathcal{F}_d(p_\xi)(t),
\]

where \( t = (t_1, t_2, \ldots, t_d) \in \mathbb{R}^d \) is the dual variable to \( y \in \mathbb{R}^d \), \( \langle y \mid t \rangle = \sum_{j=1}^{d} y_j t_j \) is the canonical inner product on \( \mathbb{R}^d \), and \( \mathcal{F}_d \) is the probabilist’s \( d \)-dimensional Fourier transform (FT) Eq. (6), may be given [10], at least approximately, as an analytical expression (similar to Eq. (3))

\[
\varphi_\xi(t) \approx \hat{\varphi}_\xi(t) = \sum_{\ell=1}^{R} \bigotimes_{\nu=1}^{d} \varphi_{\ell,\nu}(t_\nu),
\]

where the \( \varphi_{\ell,\nu}(t_\nu) \) are one-dimensional functions. Examples of such a situation are elliptically contoured \( \alpha \)-stable distributions, or also symmetric infinitely divisible distributions [10]. From this it may be deduced that an approximate low-rank expression of the pdf is given by (cf. Eq. (3))

\[
p_\xi(y) \approx \hat{p}_\xi(y) = \mathcal{F}_d^{-1}(\varphi_\xi)(y) = \sum_{\ell=1}^{R} \bigotimes_{\nu=1}^{d} \mathcal{F}_1^{-1}(\varphi_{\ell,\nu})(y_\nu),
\]
where $\mathcal{F}^{-1}_1$ is the one-dimensional probabilist’s inverse FT.

For the discrete grid $\hat{\mathbf{X}}$, there is a corresponding dual grid $\hat{\mathcal{T}} = (\hat{\mathcal{T}})_{i_0,i_1,...,i_d}$ with $1 \leq i_\nu \leq M_\nu$ for the discrete Fourier transform [16] of same size and dimensions. Similarly to the pdf evaluated on the grid $\hat{\mathbf{X}}$ and represented by the tensor $\mathbf{P}$, the pcf will be used in a setting evaluated on this dual grid $\hat{\mathcal{T}}$

$$\Phi := \varphi_\xi(\hat{\mathbf{T}}) := (\varphi_\xi(\hat{i}_{i_1,1}, \ldots, \hat{i}_{i_d,d})) = \mathcal{F}_d(\mathbf{P})$$

From Eq. (7) it is now easy to see that, as in Eq. (4), $\Phi \approx \sum_{\ell=1}^R \bigotimes_{\nu=1}^d \varphi_{\ell,\nu}$, where the vectors $\varphi_{\ell,\nu}$ are the evaluations of the one-dimensional functions $\varphi_{\ell,\nu}$ from Eq. (7), given by $\varphi_{\ell,\nu} := (\varphi_{\ell,\nu}(\hat{t}_{i_1,1}), \ldots, \varphi_{\ell,\nu}(\hat{t}_{i_M,\nu})) \in \mathbb{R}^{M_\nu}$. From these vectors $\varphi_{\ell,\nu}$ one may now compute with the discrete one-dimensional inverse Fourier transform, for the sake of simplicity again denoted by $\mathcal{F}_1^{-1}$, the vectors $\mathbf{p}_{\ell,\nu} = \mathcal{F}_1^{-1}(\varphi_{\ell,\nu})$, such that from Eq. (8) one arrives at an expression corresponding to Eq. (4):

$$\mathbf{P} = \mathcal{F}_d^{-1}(\Phi) \approx \sum_{\ell=1}^R \bigotimes_{\nu=1}^d \mathcal{F}_1^{-1}(\varphi_{\ell,\nu}) = \sum_{\ell=1}^R \bigotimes_{\nu=1}^d \mathbf{p}_{\ell,\nu}. \quad (10)$$

Thus one again obtains a numerical low-rank representation for the density as in Eq. (4). Obviously, the cross-methods [36, 99, 8, 7, 26, 31] alluded to there can be used here too, to directly obtain a low-rank representation of the pcf. Then again, with the help of the discrete inverse Fourier transforms, one arrives at a low-rank representation of the pdf.

Random vectors of high dimension $\bm{\xi}$ occur also when random fields resp. stochastic processes are discretised, often given through their so-called Karhunen-Loève expansion (KLE) [84, 67, 68] of $\bm{\xi}$, truncated at $r \in \mathbb{N}$:

$$\bm{\xi}(\omega) = \sum_{\ell=0}^r \lambda_{\ell}^{1/2} \zeta_{\ell}(\omega) \bm{v}_\ell. \quad (11)$$

This places the random vector $\bm{\xi}(\omega) = [\ldots, \xi_k(\omega), \ldots]$, a function of the two variables ($\omega, k$), in the tensor product $L_2(\Omega) \otimes \mathbb{R}^d$; and the Karhunen-Loève expansion Eq. (11) (another form of singular value decomposition) is a separated representation of this tensor of second order. Often the singular values $\lambda_{\ell}^{1/2}$ decay quickly as $\ell$ grows, so that one may obtain a good approximation with only $r$ terms.

To see in a nutshell where this leads to, assume further that the uncorrelated RVs $\zeta_{\ell}(\omega) = \sum_{\alpha} c_{\ell,\alpha} \psi_{\alpha}(\theta(\omega))$ may be expanded in Wiener’s polynomial chaos expansion (PCE), see e.g. [66], with multi-variate polynomials $\psi_{\alpha}(\theta(\omega)) := \prod_{j=1}^d \psi_{\alpha_j}(\theta_j(\omega))$ and the Karhunen-Loève expansion Eq. (11) (another form of singular value decomposition) is a separated representation of this tensor of second order. Often the singular values $\lambda_{\ell}^{1/2}$ decay quickly as $\ell$ grows, so that one may obtain a good approximation with only $r$ terms.

To see in a nutshell where this leads to, assume further that the uncorrelated RVs $\zeta_{\ell}(\omega) = \sum_{\alpha} c_{\ell,\alpha} \psi_{\alpha}(\theta(\omega))$ may be expanded in Wiener’s polynomial chaos expansion (PCE), see e.g. [66], with multi-variate polynomials $\psi_{\alpha}(\theta(\omega)) := \prod_{j=1}^d \psi_{\alpha_j}(\theta_j(\omega))$ and the Karhunen-Loève expansion Eq. (11) (another form of singular value decomposition) is a separated representation of this tensor of second order. Such a tensor can—as before—be represented in the canonical polyadic (CP) format [59], say with low $CP$-rank $R$: $\bm{Z} \approx \sum_{r=1}^R \bigotimes_{k=0}^d z_r^{(k)} = \sum_{r=1}^R z_r$.

Having $\bm{Z}$ in a low-rank representation then leads to a low-rank representation of the random vector $\bm{\xi}(\theta)$, to obtain a formula for a quick evaluation of the pcf of $\bm{\xi}(\theta)$: $\varphi_\xi(t) = \mathbb{E}(\exp(i \langle t | \bm{\xi}(\theta) \rangle_{\mathbb{R}^d}))$, yielding the pcf of $\bm{\xi}(\theta)$ in a low-rank tensor format. Now we are back to the situation as before when the pcf was assumed given.

1.2 Literature review and outline of the paper

To compute quantities of interest (QoIs) such as the $d$-divergences—see Section 3 for the distances and divergences considered—functions such as the square root, the logarithm, etc.,
have to be computed point-wise on the pdf. But in a compressed format the point values are not directly accessible. An important contribution of this paper is to show that such computations are still possible efficiently by operating directly on the compressed format. This will be enabled by identifying both the pcf and the pdf as elements of algebras. A similar idea was already used in [33, 39] for post-processing low-rank representations of RVs, and here it is extended to densities and characteristic functions. It is well-known that algebras can be represented as linear operators resp. matrices in the finite-dimensional case (e.g. [109]), and one can employ the spectral calculus of linear operators in order to obtain these point-wise evaluations in a low-rank format. In the concrete case here this boils down to using algorithms which were developed to compute functions of matrices [64].

Therefore, special compressed / low-rank data structures are needed. The CP format used above for illustrative purposes may be the simplest, but we suggest to use the low-rank tensor train (TT) data format [99, 100]. Other known tensor formats, such as: Tucker, and hierarchical Tucker (HT) could be also applied [55, 70, 75, 12]. For the sake of simplicity of exposition, the CP tensor format is considered in the main part of the paper for illustrative purposes, when direct reference to a low-rank format is necessary. The computations are also possible in other compressed formats. In [39] the computations of the operations of the algebra were already given for various tensor formats, and they may also be found e.g. in [55, 70, 75, 12], so that we may be brief here. For numerical experiments we use the Tensor Train (TT) software library TT-tool [100].

In this work we would like to explore the usefulness and applicability of these techniques in probability. In probability theory, given a $d$-dimensional RV, it is well known that its characterisation is provided by the pcf [86] (Feller and Lévi theorems). Therefore, our contribution will also focus on approximation techniques for representing the pcf in low-rank tensor format. Previous approaches to approximate the pcf were not able to handle high-dimensional RVs, e.g. [86, 110, 120]. Our approach can overcome these difficulties. Other numerical methods which rely on the use of the pcf may also benefit from the proposed approach; e.g. the idea to use Markov Chain Monte Carlo (MCMC) methods in the Fourier domain to sample from a density proportional to the absolute value of the underlying characteristic function is presented in [10].

In a very recent paper [103], the authors estimate tensor train (TT) ranks for approximated multivariate Gaussian pdfs. In [30], the authors use the TT-format to approximate multivariate probability distributions. There they analyse properties of the obtained low-rank approximation and use it as a prior distribution in the MCMC approach. In [120, 121], the author develops a numerical inversion of characteristic functions.

Low-rank tensor techniques proved to be very successful in such areas as numerical mathematics [39, 33, 80, 75, 55, 12], computational chemistry [70], statistics [83] and others [54]. Many known types of Green’s functions were approximated in the low-rank tensor format [75, 73, 74], which resulted in drastically reduced computational cost and storage.

General tensor formats and their low-rank approximations, in quantum physics also known as tensor networks, are described in [118, 105, 41, 93, 18, 14]. For the mathematical and numerical point of view we refer to the review [78], the monographs [59, 70, 75], and to the literature survey on low-rank approximations [54].

Some of the necessary theory is reviewed in Section 2. The discrete versions of the pdf and the pcf are represented in a compressed approximation, we propose to use low-rank tensor approximations. The discretised pdf and pcf are viewed as tensors equipped with a discrete version of the point-wise product, the so-called Hadamard product. With this product they become (commutative) $C^*$-algebras, so it is possible to define algebraically the desired functions on these tensors, and on their compressed approximation, through the use
of matrix algebra algorithms [64].

Assuming that the pdf has been represented in such an algebraic setting, in Section 3 we explain how to compute statistical moments and divergences in this discretised framework, using only the abstract discrete operations, independent of any particular representation. In Section 4 we show as an example how the algebraic operations may be actually implemented on a low-rank tensor format, namely first for illustrative purposes on the simpler canonical polyadic (CP) tensor decomposition, where we recall all required definitions and properties. This tensor format is the easiest one to explain the ideas. In the example computations later in Section 6 we actually use the tensor-train (TT) format, but here the explanation is more complicated. The actual algorithms—developed for matrices—which can be used to compute various functions of pdfs are either iterations or truncated series expansions, and are listed in Section 5. Again, only the abstract discrete operations are needed, and the algorithms are independent of any particular representation. In Section 6 some numerical examples are given, and Section 7 concludes.

2 Theoretical background

The two entities we will be working with are the probability density function (pdf) and the corresponding probability characteristic function (pcf). These are connected by the Fourier transform. The ultimate goal is to use discretised versions of these two descriptors of RVs to compute for example the pdf of a mixture model or the pdf of the sum of two independent RVs, or quantities of interest (QoIs) like moments, or other statistics like the relative entropy of a RV, or—for two pdfs—their Kullback-Leibler (KL) or more general f-divergences. While introducing the notation, this section serves to collect the basic properties of the different descriptors such as moments, cumulative distribution function cdf, pdf, pcf, second characteristic or cumulant generating function \[ \tilde{F} \] and low-rank representation. In the example computations on a low-rank tensor format, namely first for illustrative purposes on the simpler canonical polyadic (CP) tensor decomposition, where we recall all required definitions and properties.

2.1 Notation and summary of basic descriptors

The random vector \( \xi : \Omega \to \mathcal{V} = \mathbb{R}^d \) as a measurable mapping w.r.t. the Borel-\( \sigma \)-algebra \( \mathfrak{B}(\mathbb{R}^d) \) on \( \mathbb{R}^d \), defined on a probability space \( (\Omega, \mathfrak{A}, \mathbb{P}) \), where \( \mathfrak{A} \) is a \( \sigma \)-algebra and \( \mathbb{P} \) a

probability measure was already introduced in Section 1. We are mainly interested in the case where \( \mathcal{V} = \mathbb{R}^d \) is a high-dimensional vector space. The associated expectation operator is denoted by \( \mathbb{E} (\cdot) \), the mean as \( \mathbb{E} (\xi) = \int_{\Omega} \xi (\omega) \mathbb{P}(d\omega) \in \mathbb{R}^d \), and the mean zero random part as \( \xi := \xi - \bar{x} \). The canonical Euclidean inner product \( \langle x | y \rangle_\mathcal{V} := \sum_{k=1}^d x_k y_k \) on \( \mathcal{V} = \mathbb{R}^d \) is used to identify the space \( \mathcal{V} = \mathbb{R}^d \) with its dual. The usual order structure on \( \mathbb{R}^d = \mathcal{V} \) is assumed, so that \( x \leq y \) iff \( x_k \leq y_k \) for \( k = 1, \ldots, d \), resp. \( y - x \in \mathbb{R}^d_+ = \mathcal{V}_+ \), with positive cone \( \mathbb{R}^d_+ = \mathcal{V}_+ = \{ x \in \mathbb{R}^d \mid x_1 \geq 0, \ldots, x_d \geq 0 \} \).

The moments \( X_k \) and the central moments \( \Xi_k \) of \( \xi \) of order \( k \in \mathbb{N}_0 \) —assuming they exist—are basic descriptors of a RV and are denoted as

\[
X_k = \mathbb{E} (\xi^{\otimes k}) \in (\mathbb{R}^d)^{\otimes k}, \quad \Xi_k = \mathbb{E} (\tilde{\xi}^{\otimes k}) \in (\mathbb{R}^d)^{\otimes k}.
\]

where for \( x \in \mathbb{R}^d \) one sets \( x^{\otimes k} = \bigotimes_{j=1}^k x \). The second central moment—the covariance
matrix—is also denoted as $\Sigma_\xi = \text{cov} \xi = X_2 - \bar{\xi} \otimes \bar{\xi} \in V \otimes V = (\mathbb{R}^d)^{\otimes 2}$. If $\eta$ is another random vector with values in $\mathcal{U} = \mathbb{R}^n$, the mixed and mixed central moments are denoted by

$$
Y_{k,l} = \mathbb{E} \left( \xi^{\otimes k} \otimes \eta^{\otimes l} \right) \quad \text{and} \quad \mathcal{T}_{k,l} = \mathbb{E} \left( \tilde{\xi}^{\otimes k} \otimes \tilde{\eta}^{\otimes l} \right) \in (\mathbb{R}^d)^{\otimes k} \otimes (\mathbb{R}^n)^{\otimes l}.
$$

(13)

The covariance is also denoted as $\text{cov}(\xi, \eta) = \mathcal{T}_{1,1} = Y_{1,1} - \bar{\xi} \otimes \bar{\eta} \in V \otimes \mathcal{U} = \mathbb{R}^d \otimes \mathbb{R}^n$.

The distribution measure $P_\xi$ of $\xi$ for a Borel subset $\mathcal{E} \subseteq \mathbb{R}^d$ is as usual the push-forward $\xi_* P$ of the original measure $P$: $P_\xi(\mathcal{E}) := \xi_* P(\mathcal{E}) := P(\xi^{-1}(\mathcal{E})) = \mathbb{E}(\mathbb{1}\xi(\xi))$, where the characteristic indicator function $\mathbb{1}_\xi(y)$ is unity if $y \in \mathcal{E}$ and vanishes otherwise, and is assumed absolutely continuous w.r.t. Lebesgue measure on $\mathbb{R}^d$. This leads to an absolutely continuous cumulative distribution function (cdf) of $\xi$—defined for $y \in \mathbb{R}^d = \mathcal{V}$ via semi-infinite intervals $\mathcal{E}_y = X_{k=1}^{\infty}, y_k \in \mathcal{B}(\mathbb{R}^d)$ as

$$
F_\xi(y) := P_\xi(\mathcal{E}_y) = P(\xi \leq y) = \mathbb{E}\left(\mathbb{1}_{\xi_\leq y}(\xi)\right).
$$

(14)

The well known properties of $F_\xi$ such as positivity $F_\xi(y) \geq 0$, and the monotonicity $F_\xi(y_1) \leq F_\xi(y_2)$ for $y_1 \leq y_2$, as well as $F_\xi(y) \to 0$ as $y \to -\infty$ and $F_\xi(y) \to 1$ as $y \to +\infty$, should be replicated in any discretised setting. As $P_\xi$ is absolutely continuous, it has a Radon-Nikodým derivative $p_\xi(y) = dP_\xi/ dy \in L_1(\mathbb{R}^d, \mathbb{R})$ w.r.t. Lebesgue measure, the probability density function (pdf):

$$
p_\xi(y) = \frac{d}{dy} F_\xi(y) = \frac{\partial}{\partial y_1 \ldots \partial y_d} F_\xi(y); \quad \text{with} \; p_\xi \geq 0, \quad \text{and} \int_{\mathbb{R}^d} p_\xi(x) \; dx = 1.
$$

(15)

These defining relations for the pdf are directly implied by the properties of the cdf $F_\xi$, and are important to be preserved under discretisation and compressed low-rank approximation. The positivity in Eq. (15) means that geometrically speaking densities are in the positive convex cone of $L_1(\mathbb{R}^d, \mathbb{R})$, and the integral relation means that they lie on a hyperplane. The intersection of these two closed convex sets is denoted by

$$
\mathcal{D} := \{ p \mid p \geq 0 \} \cap \{ p \mid \int_{\mathbb{R}^d} p(x) \; dx = 1 \} \subset L_1(\mathbb{R}^d, \mathbb{R}), \quad \text{closed and convex.}
$$

(16)

In addition one notes that $\|p_\xi\|_1 := \int_{\mathbb{R}^d} |p_\xi(x)| \; dx = 1$, i.e. $p_\xi$ is on the unit sphere. Convexity of $\mathcal{D}$ in Eq. (16) means that convex combinations of densities $p_{\xi_1}, \ldots, p_{\xi_m} \in \mathcal{D}$ are again densities; corresponding to mixture models.

Direct quantities of interest (QoIs) are usually expected values of functions of $\xi$, i.e. quantities like $g = \mathbb{E}(g(\xi)) \in \mathbb{R}^m = \mathcal{Y}$. Obviously the moments and central moments Eq. (12) are special cases of this by taking as QoI $g_k : x \mapsto x^{\otimes k}$, as is the characteristic function Eq. (6). These quantities may alternatively be computed by integrating over the pdf $p_\xi$ and $\mathbb{R}^d$, like Eq. (1) in Section 1:

$$
g = \mathbb{E}(g(\xi)) = \int_{\mathbb{R}^d} g(x) \; dF_\xi(x) = \int_{\mathbb{R}^d} g(x)p_\xi(x) \; dx =: \mathbb{E}_{p_\xi}(g) \in \mathcal{Y}.
$$

(17)

As is well known (e.g. [109]), the Banach space $L_1(\mathbb{R}^d, \mathbb{R})$ is a commutative Banach algebra when the space is equipped with the convolution product:

$$
(p * q)(y) := \int_{\mathbb{R}^d} p(y - x)q(x) \; dx, \quad \text{for} \; p, q \in L_1(\mathbb{R}^d, \mathbb{R}).
$$

(18)

Observe that if $p$ and $q$ are density functions, so is $p * q$. This reflects the well known fact that if $p_\xi$ is the density of the RV $\xi$, and $p_\eta$ is the density of the independent RV $\eta$, then
$p_{\xi} * p_{\eta}$ is the density of the RV $\xi + \eta$. It also means that the closed convex set $\mathcal{D}$ in Eq. (16) is stable under convolution.

The characteristic function (pcf) of the RV $\xi$ stated already in Eq. (6) may be seen defined as a QoI via Eq. (17) with $g_t(x) = \exp(i \langle t \mid x \rangle)$, i.e. the probabilist’s Fourier transform—in other fields this is considered as the non-unitary version of the inverse Fourier transform $[\mathcal{F}]$—of the pdf. Well known $[86, 120]$ facts about characteristic functions $\varphi_{\xi} : \mathbb{R}^d \rightarrow \mathbb{C}$ are that they are bounded and uniformly continuous—$\varphi_{\xi} \in C_{bu}(\mathbb{R}^d, \mathbb{C})$—and satisfy $|\varphi_{\xi}(t)| \leq \varphi_{\xi}(0) = 1$ for all $t \in \mathbb{R}^d$, i.e. $\|\varphi_{\xi}\|_{\infty} = 1$. These conditions mean that pcf s lie on a hyperplane in the vector space $C_{bu}(\mathbb{R}^d, \mathbb{C})$, obviously reflecting the hyperplane condition—unit integral—for the pdf.

The pcf is a complex-valued function, but as the Fourier transform of the real and positive pdf, it has to satisfy some further constraints. To be able to properly formulate this, one defines an anti-linear involution or $\star$-operation $\ast$ as $\varphi_{\xi}(t) := \overline{\varphi_{\xi}(-t)}$, where the overbar denotes the complex conjugate. Now, as the pdf $p_{\xi}$ in Eq. (6) is a real function, this implies $[16, 86]$ that $\varphi_{\xi}$ is Hermitean, i.e. invariant w.r.t. the conjugation induced by the $\ast$-involution; so it satisfies $\varphi_{\xi}(t) = \overline{\varphi_{\xi}(-t)} = \varphi_{\xi}(t)$. This real subspace of Hermitean functions will be denoted by $\mathcal{H} \subset C_{bu}(\mathbb{R}^d, \mathbb{C})$.

As is well known $[109]$, the Banach space $C_{b}(\mathbb{R}^d, \mathbb{C})$ together with point-wise multiplication and the $\ast$-operation is a commutative $C^*$-algebra, and the real subspace $\mathcal{H}$ of Hermitean functions is a real sub-algebra. As $p_{\xi}$ is non-negative $[86]$, the pcf $\varphi_{\xi}$ has to be a positive definite function: for any $n \in \mathbb{N}$ and distinct points $\{t_k \in \mathbb{R}^d\}_{k=1}^n$, the matrix $\Phi_{\xi} = (a_{ij})_{i,j} \in \mathbb{C}^{n \times n}$ is Hermitean positive semi-definite in $\mathbb{C}^n$. The positive definite functions form a convex cone in $\mathcal{H}$, reflecting the positivity of the pdf. These conditions will not be so easy to directly ascertain on a discretised and compressed low-rank representation of $\varphi_{\xi}$, and are simpler checked on the pdf $p_{\xi}$. All this means that the pcf is in the intersection of this cone $\mathcal{H}$ and the hyperplane of functions with unit value at the origin in $\mathcal{H}$, again a closed and convex set, denoted by

$$\mathcal{C} = \mathcal{H} \cap \{ \varphi \mid \varphi(0) = 1 \} \cap \{ \varphi \mid \varphi \text{ is positive semi-definite} \} \subset C_{bu}(\mathbb{R}^d, \mathbb{C}).$$  \hspace{1cm} (19)

Thus, real convex combinations of pcf s are again pcf, namely of mixture models, reflecting the analogous property for pdfs in $\mathcal{D}$ in Eq. (16).

It is also easily seen that the point-wise product of two pcf s is again a pcf, and hence the set $\mathcal{C}$ in Eq. (19) is stable under point-wise products. This reflects the fact that the point-wise product $\varphi_{\xi} \cdot \varphi_{\eta}$ of the pcf s of two independent RVs $\xi$ and $\eta$ is just the pcf of their sum. This is the analogue to the previous statement about the convolution of two pdfs, showing that $\mathcal{F}_d(\mathcal{D}) \subseteq \mathcal{C}$.

### 2.2 Relations through the Fourier transform

The Fourier transform is known $[16, 86]$ to connect the algebraic convolution structure on probability densities described previously with the corresponding multiplication structure on characteristic functions. Let $p, q \in L_1(\mathbb{R}^d, \mathbb{R})$ be integrable real-valued functions in the convolution Banach-algebra, and denote their Fourier transforms (FT in Eq. (6)) by $\phi = \mathcal{F}_d(p), \psi = \mathcal{F}_d(q) \in \mathcal{H}$ (as $p, q$ are real, their FT is Hermitean), then the Fourier transform and its inverse $\mathcal{F}_d^{-1}$ has the following well known $[16, 86]$ property:

$$\mathcal{F}_d(p * q) = \mathcal{F}_d(p) \cdot \mathcal{F}_d(q) = \phi \cdot \psi \quad \Leftrightarrow \quad p * q = \mathcal{F}_d^{-1}(\phi \cdot \psi).$$  \hspace{1cm} (20)

Thus the Fourier transform (FT) is a real algebra homomorphism between the real convolution Banach-algebra $L_1(\mathbb{R}^d, \mathbb{R})$ and the real multiplication algebra $\mathcal{H}$ of Hermitean functions.
In our context, further well known [16, 109] properties of the FT, which will be needed later, are embodied in the statement $\mathcal{F}_d(\mathcal{D}) \subseteq \mathcal{C}$ at the end of Subsection 2.1, can be summarised as follows: there is a correspondence between real-valued functions in $L_1(\mathbb{R}^d, \mathbb{R})$ and Hermitean Fourier transforms $\mathcal{H}$, and the positive convex cone in $L_1(\mathbb{R}^d, \mathbb{R})$ corresponds to the convex cone of positive-definite functions in $\mathcal{H}$, while the hyperplane with unit integral in $L_1(\mathbb{R}^d, \mathbb{R})$ corresponds with the hyperplane with unit value at the origin in $\mathcal{H}$. These relations will be used in the discretised low-rank setting in the following Subsection 2.3 to ascertain the correctness of the approximations. This means that as the $pdf$ satisfies $p_k \in \mathcal{D}$ in Eq. (16), so the discretised version will have to satisfy a similar discrete constraint, and dually, as the $pcf$ satisfies $\varphi_\xi \in \mathcal{C}$ in Eq. (19), the discretised version of this quantity will have to satisfy a similar discrete constraint.

Another well known property [16, 109] of the Fourier transform that will be needed is how it connects derivatives and multiplication by the co-ordinates. We assume that all derivatives appearing in the sequel exist and are well defined. In fact, from Eq. (6) one immediately sees that $(-i \partial_\xi) \varphi_\xi(t) = \int_{\mathbb{R}^d} \overline{x_k} \exp(i \langle t, x \rangle) p_\xi(x) \, dx = \mathcal{F}_d(x_k p_\xi(x)) (t)$. Further, denoting the tensor of $k$-th derivatives by $D^k \varphi_\xi(t) = \frac{\partial^k}{\partial x_{i_1} \cdots \partial x_{i_k}} \varphi_\xi(t)$, one obtains the well-known relation

$$
(-i)^k D^k \varphi_\xi(0) = \int_{\mathbb{R}^d} x^{\otimes k} p_\xi(x) \, dx = \mathcal{F}_d \left( x^{\otimes k} p_\xi(x) \right)(0) = X_k, \quad k \in \mathbb{N}_0.
$$

(21)

Similar relations as Eq. (21) can be obtained by other characterising functions. The second characteristic function [86] —sometimes also labeled as cumulant generating function (cf. Eq. (25)) —whose derivative tensors of order $k$ are essentially the cumulants $K_k$ of $\xi$, is defined as the point-wise logarithm of the $pcf$:

$$
\chi_\xi(t) := \log(\varphi_\xi(t)) = \log \left( \mathbb{E} \left( \exp(i \langle t, \xi \rangle) \right) \right), \quad \text{with } (-i)^k D^k \chi_\xi(0) =: K_k, \quad k \in \mathbb{N}_0.
$$

(22)

The relations Eq. (21) and Eq. (22) involve the slightly annoying imaginary unit. To stay with completely real functions one may switch from the Fourier transform in Eq. (6) or Eq. (22) to the Laplace transform, at the price of working with functions which may not be defined for all $t \in \mathbb{R}^d$, but maybe only in a small neighbourhood around $0 \in \mathbb{R}^d$. The moment generating function is defined as [86] essentially the reflected Laplace transform of the density, or as evaluation of the $pcf$ Eq. (6) for purely imaginary arguments:

$$
M_\xi(t) := \mathbb{E} \left( \exp(i \langle t, \xi \rangle) \right) = \int_{\mathbb{R}^d} \exp(i \langle t, x \rangle) p_\xi(x) \, dx = \mathcal{L}_d(p_\xi)(-t) = \varphi_\xi(-i t),
$$

(23)

where $\mathcal{L}_d(p_\xi)(t) = \int \exp(-\langle t, x \rangle) p_\xi(x) \, dx$ is the two-sided $d$-dimensional Laplace transform of $p_\xi$. As in Eq. (21), one obtains

$$
D^k M_\xi(0) = \int_{\mathbb{R}^d} x^{\otimes k} p_\xi(x) \, dx = X_k, \quad k \in \mathbb{N}_0.
$$

(24)

Closely related is the cumulant generating function [86], the point-wise logarithm of the moment generating function $M_\xi$ in Eq. (23):

$$
K_\xi(t) := \log(M_\xi(t)) = \log \left( \mathbb{E} \left( \exp(i \langle t, \xi \rangle) \right) \right), \quad \text{with } D^k K_\xi(0) = K_k, \quad k \in \mathbb{N}_0.
$$

(25)

2.3 Grid functions as tensors and algebras on them

It was already pointed out in Section 1 that we want to discretise both the $pdf$ and the $pcf$, by representing them on a discrete and finite grid. We start with the $pdf$. The first thing
usually to do is to centre everything around the mean \( \bar{\xi} \) of the RV \( \xi \), i.e. to shift co-ordinates on \( \mathbb{R}^d \) by \( x \mapsto x - \bar{\xi} \). Another way of saying this is to state that we work with the centred RV \( \bar{\xi} \). We assume from now implicitly that this has been done. The values of the RV \( \xi \) and hence the support of its pdf will thus be around the origin \( 0 \in \mathbb{R}^d \).

The fully discrete representation of the pdf and the pcf is based on equi-distant grid vectors \( \hat{x}_{i_1, \ldots, i_d} = \hat{x}_{1, \ldots, d} + (i_1 - 1) \Delta x_1 \) (with increment \( \Delta x_\nu \)) of size \( M_\nu \) in each dimension \( 1 \leq \nu \leq d \) of \( \mathbb{R}^d \), which were introduced in Subsection 1.1. The whole grid was denoted by \( X = \times_{\nu=1}^d X_\nu \), and we assume that it covers the support of \( p_\nu(x) \). Observe that functions are implicitly assumed to be periodic [16] when using the FFT, hence the total \( d \)-dimensional volume covered is \( V = \prod_{\nu=1}^d M_\nu \Delta x_\nu \), and the integration rule is implicitly the iterated trapezoidal rule on a periodic grid, so each point carries the same integration weight \( 1/V \).

As already defined in Eq. (2) in Section 1, the notation \( P := p_\xi(\hat{X}) \) denotes the tensor \( P \in \bigotimes_{\nu=1}^d \mathbb{R}^{M_\nu} =: \mathcal{T} \), a finite dimensional space with \( \dim \mathcal{T} = \prod_{\nu=1}^d M_\nu =: N \), the components of which are the evaluation of the pdf \( p_\nu \) on the grid \( \hat{X} \), and similarly for any other scalar function \( f(x) \) on \( \mathbb{R}^d \). Similarly, any vector valued function \( g : \nu \rightarrow \mathbb{R}^m =: \mathcal{Y} \), when evaluated on the grid \( \hat{X} \), may be viewed as a tensor \( g(\hat{X}) \in \mathcal{Y} \otimes \mathcal{T} \), and the grid itself \( \hat{X} \) can be seen as an \( \mathbb{R}^d \) valued functions evaluated on the grid.

To achieve a similar discrete representation of the pcf, it was mentioned in Subsection 1.1 that one makes use of Eq. (9), \( \Phi = \mathcal{F}_d(P) \), a discrete version of the relation Eq. (6), denoting the discrete \( d \)-dimensional Fourier transform on the grid \( \hat{X} \) again by \( \mathcal{F}_d \) for the sake of simplicity. For the dual grid \( \tilde{T} = \times_{\nu=1}^d \tilde{T}_\nu \) from Subsection 1.1, the dual grid vector in each dimension is \( \tilde{T}_\nu := (\tilde{t}_{1,\nu}, \ldots, \tilde{t}_{M_\nu,\nu}) \). As is well known [16], if in dimension \( \nu \) one has \( L_\nu = M_\nu \Delta x_\nu \), as period length for the equi-distantly spaced primal grid with grid spacing \( \Delta x_\nu \), then \( \tilde{t}_{M_\nu,\nu} = \pi/\Delta x_\nu \) is the highest (Nyquist) frequency, and the equi-distant spacing of the dual grid in dimension \( \nu \) is \( 2\pi/L_\nu \). It is assumed that the origin \( 0 \in \mathbb{R}^d \) is in the dual grid, \( 0 \in \tilde{T} \), and we denote the index of the origin in the grid with \( j^0 = (j_{1}^{0}, \ldots, j_{d}^{0}) \), i.e. \((\tilde{t}_{1,1}^{0}, \ldots, \tilde{t}_{d,d}^{0}) = 0 = (0, \ldots, 0) \). This point will be important in some of the statistics resp. Qols to be described later in Section 3. As before, the whole grid can be seen as an order \( (d+1) \) tensor \( \tilde{T} \in \mathbb{R}^d \otimes \mathcal{T} = \mathcal{V} \otimes \mathcal{T} \). The pcf on the dual grid is represented as in Eq. (9) through the tensor \( \Phi := \phi_\xi(\tilde{T}) \in \mathcal{T} \). It is on these grid representations \( P := p_\xi(\hat{X}) \) of the pdf and \( \Phi := \phi_\xi(\tilde{T}) \) of the pcf that we propose to operate on to compute the desired quantities of interest, e.g. the differential entropy Eq. (1) in Section 1. A more comprehensive list of such quantities of interest is given in Section 3.

It was already noted that even for modest values of dimension \( d \) and number of discretisation points \( n \) the total amount of data \( N = n^d \) may become huge or even non-manageable, and one has to resort to some kind of compressed representation resp. approximation. Here we advocate for low-rank tensor representations to allow for efficient computation, which will be treated in Section 4. In such a representation it becomes difficult to compute point-wise functions (like the log) of values of particular tensors required for particular statistics (cf. Section 3), as they are not accessible directly. To still be able to do these computations, we will rely on certain algebraic properties, cf. Section 5. These algebraic relations have been pointed out for the non-discrete entities in the preceding Subsection 2.2, as well as the rôle of the Fourier transform in connecting them. It is now important to ascertain that such algebraic relations also hold for the grid-discrete quantities.

The set of tensors for the representations of pdf and pcf, \( \mathcal{T} = \bigotimes_{\nu=1}^d \mathbb{R}^{M_\nu} \cong \mathbb{R}^N \) is clearly a vector space. The Section 4 will explain how the vector operations can be numerically performed in the low-rank representation. This assures that convex linear combinations of different pdfs or pcf can be computed. Furthermore, one makes \( \mathcal{T} \) into a Euclidean space
by extending the canonical inner products on the $\mathbb{R}^{M_\nu}$ onto $\mathcal{T}$; i.e. for elementary tensors $r = \bigotimes_{\nu=1}^d r_\nu, s = \bigotimes_{\nu=1}^d s_\nu, \in \mathcal{T}$, it is simply $(r | s)_{\mathcal{T}} := \prod_{\nu=1}^d (r_\nu | s_\nu)_{\mathbb{R}^{M_\nu}}$, and then extended to all of $\mathcal{T}$ by linearity.

It is convenient to extend this inner product to larger tensor products [55], and only perform a partial inner product. For example, if $S = y \otimes r$ is an elementary tensor in $\mathcal{Y} \otimes \mathcal{T}$, and $u \in \mathcal{T}$, then the partial product, denoted as before, is $(S | u)_{\mathcal{T}} := (y \otimes r | u)_{\mathcal{T}} = (r | u)_\mathcal{T} y \in \mathcal{Y}$, and then extended to all of $\mathcal{Y} \otimes \mathcal{T}$ by linearity. It is practically a contraction over all indices related to $\mathcal{T}$.

The next task is to introduce the algebraic structures. For $r = (r_1, \ldots, r_{M_\nu}), s = (s_1, \ldots, s_{M_\nu}) \in \mathbb{R}^{M_\nu}$, we want to define the circular convolution $z := (z_1, \ldots, z_{M_\nu}) = r \ast s \in \mathbb{R}^{M_\nu}$ component-wise as $z_k := \sum_{\ell=1}^{M_\nu} r_\ell s_m$, $m = ((k - \ell) \mod M_\nu) + 1; 1 \leq k \leq M_\nu$ [16, 55]. This is an associative and commutative product; the convolution algebra on $\mathbb{R}^{M_\nu}$. It is the discrete version of the convolution algebra $L_1(\mathbb{R}^d, \mathbb{R})$ considered in Subsection 2.2. One should point out [16] that two steps are involved in going from $\mathbb{R}^d$ resp. $\mathbb{R}$ to the finite grids $\tilde{X}$ resp. $\tilde{x}$: One is the truncation of the infinite domain, say $\mathbb{R}$ in dimension $\nu$, to a finite one—the interval $[\xi_{\nu}^{(\text{min})}, \xi_{\nu}^{(\text{max})}]$. This picks only certain discrete frequencies or wavenumbers [16] from the continuum in the Fourier transform, and they are all multiples of a basic frequency resp. wavenumber. The second step is the use of a finite grid, this picks a finite number of the discrete frequencies. The effect of this is to make everything implicitly periodic, through periodic continuation. This is reflected in the use of the circular convolution.

Having defined the circular convolution on each $\mathbb{R}^{M_\nu}$, it is defined on $\mathcal{T} = \bigotimes_{\nu=1}^d \mathbb{R}^{M_\nu}$ first via elementary tensors $r = \bigotimes_{\nu=1}^d r_\nu, s = \bigotimes_{\nu=1}^d s_\nu \in \mathcal{T}$ as $z = r \ast s := \bigotimes_{\nu=1}^d r_\nu \ast s_\nu$, and extended to all of $\mathcal{T}$ by linearity. This again is an associative and commutative product; the convolution algebra on $\mathcal{T}$. In passing one may remark that the statement that the discrete version $\Phi$ of the pcf is Hermitian positive definite is equivalent with the statement that the linear (in $r$) operator $K_\Phi : r \mapsto \Phi \ast r$ is Hermitian or self-adjoint and positive definite; $K_\Phi$ is the operator of convolution with $\Phi$.

The discrete version of the pointwise product is the Hadamard product, and again first formulated component-wise on $\mathbb{R}^{M_\nu}$: For $r = (r_1, \ldots, r_{M_\nu}), s = (s_1, \ldots, s_{M_\nu}) \in \mathbb{R}^{M_\nu}$ it is denoted by [55] $z := (z_1, \ldots, z_{M_\nu}) = r \circ s \in \mathbb{R}^{M_\nu}$ and defined component-wise as $z_k := r_k \cdot s_k$, $1 \leq k \leq M_\nu$. This also is an associative and commutative product; the Hadamard algebra on $\mathbb{R}^{M_\nu}$. It is again defined to $\mathcal{T} = \bigotimes_{\nu=1}^d \mathbb{R}^{M_\nu}$ via elementary tensors $r = \bigotimes_{\nu=1}^d r_\nu$ and $s = \bigotimes_{\nu=1}^d s_\nu \in \mathcal{T}$ as $z = r \circ s := \bigotimes_{\nu=1}^d r_\nu \circ s_\nu$, and extended to all of $\mathcal{T}$ by linearity. And again this is an associative and commutative product; the Hadamard algebra on $\mathcal{T}$. The interaction with the inner product is quite simple, it is an elementary calculation to verify that for $w, r, s \in \mathcal{T}$ $(w \circ r | s)_{\mathcal{T}} = (r | w \circ s)_{\mathcal{T}}$, which means that the linear (in $r$) operation of Hadamard multiplication by $w$, i.e. $L_w : r \mapsto w \circ r$, is self-adjoint.

It is easily seen that the Hadamard algebra has a multiplicative unit, which we denote by $1 = (1_{i_1}, \ldots, 1_{i_d})$ — the tensor with all ones — satisfying $r \circ 1 = r$ for any $r \in \mathcal{T}$. Defining $1_\nu := (1, \ldots, 1) \in \mathbb{R}^{M_\nu}$, a vector of all ones in dimension $\nu$ (which is the Hadamard unit for the Hadamard algebra on $\mathbb{R}^{M_\nu}$), it is not difficult to see that the Hadamard unit on the tensor product has rank one: $1 = \bigotimes_{\nu=1}^d 1_\nu$; it is the simple tensor product of the Hadamard units on each $\mathbb{R}^{M_\nu}$.

The unit further allows to introduce a discrete expectation or integral operator. Recall that we have a tensor quadrature grid, equi-spaced in each dimension, in order to use the FFT. As mentioned before, each point has the integration weight $V_N$. Hence for a tensor $P$, representing a function $p(x)$ evaluated on the grid, the approximate integral is

$$\int p(x) \, dx \approx S(P) := \frac{V}{N} (P | 1)_{\mathcal{T}}. \quad (26)$$
Eq. (26) is only a convenient way of writing the approximate integral, and obviously there
is no need to actually compute the inner product with \( \mathbf{1} \), i.e. multiply each entry in the
low-rank representation of \( \mathbf{P} \) with unity. This Eq. (26) can be simply extended to discrete
integrands of the form \( \mathbf{S} \in \mathcal{Y} \otimes \mathcal{T} \) through the use of the partial inner product defined above
with the result \( S(\mathbf{S}) \in \mathcal{Y} \). If \( \mathbf{F} \) is a tensor which represents the grid-values of a function
\( f(x) \), i.e. \( \mathbf{F} = f(\mathbf{X}) \), and \( \mathbf{P} \) represents the pdf \( p_x \), one may define a discrete version of the
expectation, which can be extended to other tensors \( \mathbf{S} \in \mathcal{Y} \otimes \mathcal{T} \), by

\[
\mathbb{E}(f(\xi)) = \mathbb{E}_{p_x}(f) = \int_{\mathbb{R}^d} f(x)p_x(x) \, dx \approx S(\mathbf{F} \odot \mathbf{P}) = \frac{1}{N} (\mathbf{F} \mid \mathbf{P})_{\mathcal{T}} =: \mathbb{E}_p(\mathbf{F}). \tag{27}
\]

To translate the statements in Subsection 2.2 into the present discrete setting, let \( \mathbf{p}, \mathbf{q} \in \mathcal{T} \)
be two tensors, and \( \Phi = \mathcal{F}_d(\mathbf{p}), \Psi = \mathcal{F}_d(\mathbf{q}) \in \mathcal{T} \) their discrete Fourier transforms. Then one
has just as in Eq. (20)

\[
\mathcal{F}_d(\mathbf{p} \ast \mathbf{q}) = \mathcal{F}_d(\mathbf{p}) \odot \mathcal{F}_d(\mathbf{q}) = \Phi \odot \Psi \iff \mathbf{p} \ast \mathbf{q} = \mathcal{F}_d^{-1}(\Phi \odot \Psi), \tag{28}
\]

showing that the discrete Fourier transform (FT) is an algebra isomorphism between the
convolution algebra \( (\mathcal{T}, \ast) \) and the Hadamard algebra \( (\mathcal{T}, \odot) \). This makes it relatively easy
to compute the discrete convolution of the tensor representations of two densities, say \( \mathbf{p} \)
represented by \( \mathbf{P} \), and \( \mathbf{q} \) represented by \( \mathbf{Q} \). Then the density \( \mathbf{p} \ast \mathbf{q} \) corresponds to \( \mathbf{P} \ast \mathbf{Q} \),
computed with their Fourier transforms \( \Phi = \mathcal{F}_d(\mathbf{p}) \) and \( \Psi = \mathcal{F}_d(\mathbf{q}) \) as
\( \mathbf{P} \ast \mathbf{Q} = \mathcal{F}_d^{-1}(\Phi \odot \Psi) = \mathcal{F}_d^{-1}(\mathcal{F}_d(\mathbf{P}) \odot \mathcal{F}_d(\mathbf{Q})) \).

For a real tensor \( \mathbf{w} \), the Hadamard multiplication operator \( \mathbf{L}_w \) of Hadamard multiplica-
tion with \( \mathbf{w} \) was defined above. As the Hadamard algebra is commutative, the Hadamard
multiplication operators commute with each other. Thus it is theoretically clear \cite{109} that
they can be simultaneously diagonalised. But it is elementary to see this explicitly. If an
arbitrary tensor \( \mathbf{r} \in \mathcal{T} \) were written as a vector, the action \( \mathbf{L}_w(\mathbf{r}) = \mathbf{w} \odot \mathbf{r} \) would be the
action of a diagonal matrix, and diagonal matrices obviously commute. This means that
\( \mathbf{L}_w \) is fully diagonalised, and the components \( w_{j_1,\ldots,j_d} \) of the tensor \( \mathbf{w} \) are in fact the
diagonal elements, i.e. the eigenvalues of \( \mathbf{L}_w \). Obviously, to an eigenvalue \( w_{j_1,\ldots,j_d} \) belongs the
canonical unit vector with the same index as eigenvector, in tensor notation the eigenvector
is \( \mathbf{v}^{(j_1,\ldots,j_d)} = (\delta_{j_1,\ldots,j_d,1_1,\ldots,1_d}i_1,\ldots,i_d) \), i.e. \( \mathbf{L}_w(\mathbf{v}^{(j_1,\ldots,j_d)}) = w_{j_1,\ldots,j_d} \mathbf{v}^{(j_1,\ldots,j_d)} \).

Let \( \Phi = \mathcal{F}_d^{-1}(\mathbf{w}) \), and let \( \mathbf{r} \in \mathcal{T} \) be any tensor. The convolution operator \( \mathbf{K}_\phi \) of convolu-
tion with a Hermitian \( \Phi \) was defined above. One then has

\[
\begin{align*}
\mathbf{K}_\phi(\mathbf{r}) = \mathbf{r} \ast \mathbf{r} & = \mathcal{F}_d^{-1}((\mathcal{F}_d(\Phi) \odot \mathcal{F}_d(\mathbf{r}))) = \mathcal{F}_d^{-1}((\mathbf{w} \odot \mathcal{F}_d(\mathbf{r}))) = \mathcal{F}_d^{-1}(\mathbf{L}_w(\mathcal{F}_d(\mathbf{r}))), \quad \text{or} \quad (29) \\
\mathbf{L}_w(\mathbf{r}) & = \mathbf{w} \odot \mathbf{r} = \mathcal{F}_d(\Phi) \odot \mathbf{r} = \mathcal{F}_d((\mathbf{r} \ast \mathcal{F}_d^{-1}(\mathbf{r}))) = \mathcal{F}_d(\mathbf{K}_\phi(\mathcal{F}_d^{-1}(\mathbf{r}))). \quad \text{or} \quad (30)
\end{align*}
\]

This shows that \( \mathbf{K}_\phi \) and \( \mathbf{L}_w \) are unitarily equivalent and have the same eigenvalues; and
since those of \( \mathbf{L}_w \) are the components \( w_{j_1,\ldots,j_d} \) of the tensor \( \mathbf{w} \), those of \( \mathbf{K}_\phi \) are the same, i.e. the
components of \( \mathbf{w} = \mathcal{F}_d(\Phi) \), the Fourier transform of the Hermitian convolution tensor
\( \Phi \).

When manipulating tensors which represent discrete versions of the pdf resp. the pcf,
one wants to make sure that these manipulations do not destroy the fundamental properties
of these objects. Let us consider discrete densities first, and assume that \( \mathbf{P} \in \mathcal{T} \) is the
discrete representation of a density. Then we should expect \( \mathbf{P} \geq \mathbf{0} \), i.e. for each \( 1 \leq i_\nu \leq M_\nu \), \( 1 \leq \nu \leq d \): \( P_{i_1,\ldots,i_d} \geq 0 \). We have tacitly assumed that \( \mathbf{P} \) is also real-valued; this is
not necessarily so if it is numerically computed with the involvement of the FT. But this
condition is easy to check, as usually the real and imaginary parts of a complex tensor are
approximated separately; one only has to make sure the imaginary part is identical to zero—or even better, not computed or stored at all by using a half-length compressed real version of the FFT. This incidentally insures that its FT $\Phi = \mathcal{F}_d(P)$ is Hermitean. This condition is preserved by the discrete FT. Coming back to the positivity of $P$, this can be checked by computing its minimum component $P_{\text{min}}$; this minimum should be non-negative, making $L_P$ positive. If it happens to be negative, those components can be removed and set to zero. It will be explained later in Section 5 on how to do this. Observing this will also automatically make its FT $\Phi$ resp. $K_\Phi$ positive definite.

A further condition is that the density integrates to unity. Hence in the discrete setting we should expect $S(P) = 1$. Incidentally, if $\Phi = \mathcal{F}_d(P)$ is its FT, then this is equivalent with $\Phi^\rho = \Phi_{i_1,\ldots,i_d}^\rho = 1$. If $P$ does not meet this condition, then it can be rescaled appropriately.

The last task to address in connection with compressed resp. low-rank tensor approximations is how to compute point-wise functions $f(w)$ of a real tensor $w \in \mathcal{T}$, which means the same function applied to each component. Normally, in a full representation, this computation is no problem, but in a compressed representation the component values are not directly accessible. The Hadamard algebra can be used to accomplish this function evaluation, continuing [33, 39]. This builds theoretically on generally well known results (e.g. [109]) about the evaluation of functions of self-adjoint linear operators like $L_P$ with the spectral functional calculus, and abstractly on how to compute functions of self-adjoint elements in an Abelian C*-algebra. More specifically, as will be seen later, one may use well known algorithms for (real and self-adjoint) matrices [64] to actually do the calculations.

The simplest functions like linear combinations follow from the vector space structure of $\mathcal{T}$. The next in complexity are powers and polynomials. For $m \in \mathbb{N}_0$, the powers are defined as usual by $r^{\odot m} := r^{\odot(m-1)} \odot r$, setting $r^{\odot 0} = 1$. This way one may evaluate polynomials

$$f_p(t) = \sum_{m=0}^{M} \beta_m t^m$$

by replacing $t^m$ with $r^{\odot m}$.

The inverse function $f_i(t) = 1/t = t^{-1}$ is easy to deal with, as the existence of a unit allows the definition of an inverse element: $r \in \mathcal{T}$ is called invertible, if there exists a—unique—element $w \in \mathcal{T}$ such that $r \odot w = 1$; it is denoted by $w = r^{\odot^{-1}}$. It is obvious that for $r \in \mathcal{T}$ to have a Hadamard inverse, no component can vanish, $r_{i_1,\ldots,i_d} \neq 0$. In that case $r^{\odot^{-1}} = (1/r_{i_1,\ldots,i_d})$. This is up to now only a definition of $f_i(r) = r^{\odot^{-1}}$, and not yet an algebraic way of computing it.

Power series $f_{ps}(t) = \sum_{m=0}^{\infty} \beta_m t^m$, or more generally $f_{ps}(t) = \sum_{m=0}^{\infty} \beta_m (t - t_0)^m$ are—thanks to the Cayley-Hamilton theorem—actually polynomials on the finite dimensional Hadamard algebra—see the remarks on general functions in the following. In case $f_h$ is a holomorphic function in a complex domain containing the values of $r$, it can also be evaluated in the algebra via Cauchy’s formula: $f_h(r) = f_T f_h(z) (z \cdot 1 - r)^{\odot -1} \, dz \in \mathcal{T}$, where $T$ is a contour in $\mathbb{C}$ inside the domain of holomorphy, with all values of $r$ inside the contour.

The computation of a general function $f(r)$ —where $f$ is a real valued function defined on a subset of $\mathbb{R}$ which includes all the values of $r$—makes use of the representation $r \mapsto L_r$ from the algebra $(\mathcal{T}, \odot)$ into the algebra $(\mathcal{L}(\mathcal{T}), \circ)$ —the algebra of linear operators with concatenation “$\odot$” as multiplication. This is an injective algebra homomorphism onto an Abelian sub-algebra of $\mathcal{L}(\mathcal{T})$ of self-adjoint operators. The general way to compute a function $f(r)$ of a self-adjoint $L_r$ is to use the spectral calculus (e.g. [109]). This will work in any unital C*-algebra; it is mentioned only for general background orientation, the situation here is much simpler. We saw that the operators $L_r$ can be represented by diagonal matrices. This means that matrix algorithms, which only use the matrix algebra operations, can be used to compute $f(L_r)$ to represent $f(r)$, see e.g. [64]. The algorithms will explicitly be addressed later in Section 5, and may be used directly on the Hadamard algebra, and there is no need to actually use matrices. With that in mind, it may be mentioned in passing
that as the spectrum resp. set of eigenvalues of $L_r$ is a finite set, any function $f(r)$ could in principle be interpolated by a polynomial. But this is not practical, as the polynomial would in general have degree $N = \dim\mathcal{T}$, which we assume to be a huge number, so that typically the matrix algorithms are more economical.

3 Computation of moments and divergences

This section explains how to compute QoIs already mentioned in Section 2 from pdfs or pcfs given in compressed representation. It is thereby assumed that point-wise functions of the compressed representation resp. low-rank tensor approximation can be computed. Algorithms for this task will be shown in Section 5. Moreover, the computation of various distances and divergences between pdfs will be treated in this discrete setting, noting the point-wise functions which are required to compute them.

If it is desired to compute some QoI—the expected value of a function $g(\xi)$ (with $g : \mathbb{R}^d \rightarrow \mathcal{Y}$) of the RV $\xi$ like in Eq. (17), then it is first necessary to represent this function in low-rank format on the grid $\tilde{\mathcal{T}}$, i.e. to find $G = g(\tilde{\mathcal{X}}) \in \mathcal{Y} \otimes \tilde{\mathcal{T}}$. If $P$ represents the pdf $p_\xi$, the discrete version of the expectation was already given in Eq. (27): $E_P(G) = \frac{1}{N} \langle G | P \rangle_{\mathcal{T}}$.

Moments are a special case: for the mean one takes the tensor $\bar{x}$, or for higher moments the tensor $x \otimes k$: $\bar{\xi} = X_1 \approx E_T(x)$, and $X_k \approx E_P(x^{\otimes k})$. For mixed moments these relations can be used in an analogous fashion.

Other characterising functions were sketched at the end of Subsection 2.2. The simplest one is the second characteristic function $\chi_\xi(t) = \log(\varphi_\xi(t))$ from Eq. (22). Given the tensor $\Phi$ representing $\varphi_\xi$, this is just the point-wise logarithm $\Upsilon = \log(\Phi)$, such that $\Upsilon = \chi_\xi(\tilde{T})$. (31)

From this one may compute cumulants

$$K_k \approx \left( F_d \left( x^{\otimes k} \odot F_d^{-1}(\Upsilon) \right) \right)_{j_0}. \quad \text{(32)}$$

The moment generating function $M_\xi(t) = \mathbb{E}(\exp{\langle t | \xi \rangle})$ Eq. (23) can in principle be generated in the same way as the characteristic function $\varphi_\xi(t) = \mathbb{E}(\exp(i\langle t | \xi \rangle))$ with the help of the RV $\xi(\cdot)$ to give its tensor representation $M = M_\xi(\tilde{T})$ on the grid $\tilde{T}$. Its derivatives are directly the moments, so with the FT one has an alternative approximate computation of the moments:

$$\bar{\xi} \approx \mathbb{E}_T(x) = i \left( F_d \left( x \odot F_d^{-1}(M) \right) \right)_{j_0}, \quad \text{and}$$

$$X_k \approx \mathbb{E}_T(x^{\otimes k}) = i^k \left( F_d \left( x^{\otimes k} \odot F_d^{-1}(M) \right) \right)_{j_0}. \quad \text{(34)}$$

Similarly to the discrete version of second characteristic function Eq. (31), the cumulant generating function $K_\xi(t) = \log(M_\xi(t))$ in Eq. (25) also has a discrete version, the point-wise logarithm of the discrete moment generating function $M$:

$$Z = \log(M), \quad \text{such that } Z = K_\xi(\tilde{T}). \quad \text{(35)}$$

Analogous as before in Eq. (34), the cumulants may be expressed via

$$K_k \approx i^k \left( F_d \left( x^{\otimes k} \odot F_d^{-1}(Z) \right) \right)_{j_0}. \quad \text{(36)}$$
If the discretised pcf $\Phi$ has low tensor rank, then $X_k$ will also be of a low-rank. Note that we cannot say the same about $K_k$ from Eq. (32) (or Eq. (36)). The tensor rank of $K_k$ depends on the tensor rank of $\Upsilon$ (or $Z$), and the latter can have a high rank due to the involved $\log(\cdot)$ function. Hence it is assumed here that the series expansion described in Subsection 5.4 will allow it to approximate $\Upsilon$ (or $Z$) in a low-rank tensor format.

Table 1: List of some typical divergences and distances.

| Name of the divergence | Approximation of $D_\bullet(p\|q)$ |
|------------------------|-----------------------------------|
| Kullback–Leibler-(KL) — $D_{KL}$: | $\int (\log(p(x)/q(x))) p(x) \, dx = \mathbb{E}_p(\log(p/q))$ |
| squared Hellinger dist. — $(D_H)^2$: | $\frac{1}{2} \int \left( \sqrt{p(x)} - \sqrt{q(x)} \right)^2 dx$ |
| Bregman divergence — $D_\phi$: | $\int \left[ \phi(p(x)) - \phi(q(x)) \right] - (p(x) - q(x)) \phi'(q(x)) \, dx$ |
| Bhattacharyya distance — $D_{Bh}$: | $- \log \left( \int \sqrt{(p(x)q(x))} \, dx \right)$ |

Let us now turn to quantities which characterise the whole distribution, or the difference or distance between them. A simple characterisation of a distribution is its entropy, which was already encountered in Section 1. For a continuous distribution $p$ this is the differential entropy, requiring the point-wise logarithm of $P$:

$$h(p) := \mathbb{E}_p(-\log(p)) \approx \mathbb{E}_P(-\log(P)) = -\frac{V}{N} \langle \log(P) \mid P \rangle,$$
(37)

where the expectation $\mathbb{E}_P(\cdot)$ is computed as in Eq. (27).

Table 2: Discrete approximations for divergences listed in Table 1. Formulas for computations are given in Section 2 and Section 5.

| Name of the divergence | Approximation of $D_\bullet(p\|q)$ |
|------------------------|-----------------------------------|
| Kullback–Leibler-(KL) — $D_{KL}$: | $\frac{V}{N} \langle \log(P) \mid P \rangle - \langle \log(Q) \mid P \rangle$ |
| squared Hellinger distance — $(D_H)^2$: | $\frac{V}{2N} \langle P^{\odot^{1/2}} - Q^{\odot^{1/2}} \mid P^{\odot^{1/2}} - Q^{\odot^{1/2}} \rangle$ |
| Bregman divergence — $D_\phi$: | $\frac{V}{2N} \langle (\phi(P) - \phi(Q)) - (P - Q) \odot \phi'(Q) \rangle$ |
| Bhattacharyya distance — $D_{Bh}$: | $- \log \left( \frac{V}{N} \langle P^{\odot^{1/2}} \mid Q^{\odot^{1/2}} \rangle \right)$ |

To compare two pdfs $p$ and $q$, one uses divergences or distances between them. The best known is probably the relative entropy, also known as the Kullback-Leibler (KL) divergence. Divergences are a kind of generalisation of distances, but unlike distances they do not have to be symmetric. Let $p, q \in \mathcal{D}$ be two pdfs, and $P, Q \in \mathcal{T}$ their low-rank tensor representations. Some well known divergences and distances are given in Table 1. For the Bregman divergence, $\phi$ has to be a real convex function, e.g. $\phi(t) = t^2$. These divergences and distances may be computed by the discrete approximations shown in Table 2.
It is evident that one has to be able to compute the point-wise logarithm and the square root of a low-rank tensor. For the Bregmann divergence one has to be able to compute point-wise the convex function $\phi$ and its derivative $\phi'$ of a low-rank tensor representation, an easy task for $\phi(t) = t^2$.

The $f$-divergence is a way to define many divergences in a unifying way [82, 90], depending on a convex function $f$. One requires that $f$ be a convex function, satisfying $f(1) = 0$. Then the $f$-divergence of $p$ from $q$ and its discrete approximation is defined as

$$D_f(p||q) := \mathbb{E}_q \left( f \left( \frac{p}{q} \right) \right) \approx \mathbb{E}_Q \left( f(P \odot Q^{\odot-1}) \right) = \frac{V}{N} \left< f(P \odot Q^{\odot-1}) \mid Q \right> . \quad (38)$$

Many common divergences, such as the KL-divergence, the Hellinger distance, and the total variation distance, are special cases of the $f$-divergence, coinciding with a particular choice of $f$. In Table 3 the functions $f$ for some common $f$-divergences [82, 90] are listed.

| Name of the divergence                  | Corresponding $f(t)$                      |
|----------------------------------------|------------------------------------------|
| KL-divergence                          | $t \log(t)$                              |
| reverse KL-divergence                  | $- \log(t)$                              |
| squared Hellinger distance             | $(\sqrt{t} - 1)^2$                       |
| total variation distance               | $|t - 1|/2$                               |
| Pearson $\chi_p^2$-divergence          | $(t - 1)^2$                              |
| Neyman $\chi_N^2$-divergence (reverse Pearson) | $t^{-1} - 1$                          |
| Pearson-Vajda $\chi_P^k$-divergence   | $(t - 1)^k$                              |
| Pearson-Vajda $|\chi_P^k|$-divergence | $|t - 1|^k$                              |
| Jensen-Shannon-divergence              | $t \log(t) - (t + 1) \log((t + 1)/2)$   |

Hence to compute the discrete approximation, one has to be able to compute not only the Hadamard inverse of a low rank tensor, but also the function $f$. These are essentially the ones which have been discussed already, the only new one is the absolute value.

4 Tensor formats

In this section some well-known technical details scattered in the literature about algebraic computations in low-rank tensor formats are collected. Many tensor formats are used in quantum physics under the name tensor networks, see [118, 105, 41, 93, 18, 14]. The canonical polyadic (CP) [65] and Tucker [114] formats have been well known for a long time and are therefore very popular. For instance, CP and Tucker rank-structured tensor formats have been applied in chemometrics and in signal processing [111, 21]. The Tensor Train format was originally developed in quantum physics and chemistry as “matrix product states” (MPS), see [118] and references therein, and rediscovered and developed further in [99, 100, 7, 26] as tensor train format. The hierarchical tensor (HT) format was introduced in [58], and further considered in [51].

The CP format is cheap, it is simpler than the Tucker or TT format, but, compared to others, there are no reliable algorithms to compute CP decompositions for $d > 2$ [59, 75]. The
Tucker format has stable algorithms [74], but the storage and complexity costs are \( \mathcal{O}(drn + r^d) \), i.e. they grow exponentially with \( d \). The TT format is a bit more complicated, but does not have this disadvantage. Applications to UQ problems are described in [24, 25, 23].

The higher the order of the tensor, the more possibilities there are to find a low-rank approximation [59], as such tensors contain not only rows and columns, but also slices and fibres [77, 78, 22, 59]. These can be analysed for linear dependencies, super symmetry, or sparsity, and may result in a strong data compression [115].

### 4.1 The canonical polyadic (CP) tensor format

The CP representation of a multivariate function is one of the easiest tensor representations, it was developed in [65]. A tensor representation is a multi-linear mapping. There are many different representations, e.g., the CP tensor representation maps a tensor \( \mathbf{w} \) into a sum with \( r \) terms \( \sum_{r=1}^{d} \mathbf{w}_{i_{1},\ldots,i_{d}} \). The number \( r \) is called the tensor rank. The storage required to store a tensor in the CP tensor format is \( \mathcal{O}(r d n) \) (assuming that 2 = \( n_{1} = \ldots = n_{d} \)).

Denoting the set of all rank-\( r \) tensors by \( \mathcal{T}^{r} \), it is evident that if \( \mathbf{w}_{1},\mathbf{w}_{2} \in \mathcal{T}^{r} \), then the sum \( \mathbf{w}_{1} + \mathbf{w}_{2} \notin \mathcal{T}^{r} \), and, therefore, \( \mathcal{T}^{r} \) is not a vector space [40]. This sum is generally in \( \mathcal{T}^{2r} \).

A complete description of fundamental operations in the canonical tensor format and their numerical cost can be found in [59]. For recent algorithms in the canonical tensor format we refer to [55, 12, 35, 36, 37]. To multiply a tensor \( \mathbf{w} \) by a scalar \( \alpha \in \mathbb{R} \) costs \( \mathcal{O}(r n d) \):

\[
\alpha \cdot \mathbf{w} = \sum_{j=1}^{r} \sum_{\nu=1}^{d} \alpha_{\nu} \mathbf{w}_{j,\nu},
\]

where \( \alpha_{\nu} := \sqrt{|\alpha|} \) for all \( \nu > 1 \), and \( \alpha_{1} := \text{sign}(\alpha) \sqrt{|\alpha|} \).

The sum of two tensors costs only \( \mathcal{O}(1) \):

\[
\mathbf{w} = \mathbf{u} + \mathbf{v} = \left( \sum_{j=1}^{r_{u}} \sum_{\nu=1}^{d} \mathbf{u}_{j,\nu} \right) + \left( \sum_{k=1}^{r_{v}} \sum_{\mu=1}^{d} \mathbf{v}_{k,\mu} \right) = \sum_{j=1}^{r_{u}+r_{v}} \sum_{\nu=1}^{d} \mathbf{w}_{j,\nu},
\]

where \( \mathbf{w}_{j,\nu} := \mathbf{u}_{j,\nu} \) for \( j \leq r_{u} \) and \( \mathbf{w}_{j,\nu} := \mathbf{v}_{j,\nu} \) for \( r_{u} < j \leq r_{u} + r_{v} \). The sum \( \mathbf{w} \) generally has rank \( r_{u} + r_{v} \). The Hadamard product can be written as follows

\[
\mathbf{w} = \mathbf{u} \odot \mathbf{v} = \left( \sum_{j=1}^{r_{u}} \sum_{\nu=1}^{d} \mathbf{u}_{j,\nu} \right) \odot \left( \sum_{k=1}^{r_{v}} \sum_{\mu=1}^{d} \mathbf{v}_{k,\mu} \right) = \sum_{j=1}^{r_{u}} \sum_{k=1}^{r_{v}} \sum_{\nu=1}^{d} \left( \mathbf{u}_{j,\nu} \odot \mathbf{v}_{k,\nu} \right).
\]

The new rank can increase till \( r_{u} r_{v} \), and the computational cost is \( \mathcal{O}(r_{u} r_{v} n d) \). The scalar product can be computed as follows:

\[
\langle \mathbf{u} | \mathbf{v} \rangle_{\mathcal{T}} = \left( \sum_{j=1}^{r_{u}} \sum_{\nu=1}^{d} \mathbf{u}_{j,\nu} \right) \left( \sum_{k=1}^{r_{v}} \sum_{\mu=1}^{d} \mathbf{v}_{k,\mu} \right) = \sum_{j=1}^{r_{u}} \sum_{k=1}^{r_{v}} \prod_{\nu=1}^{d} \langle \mathbf{u}_{j,\nu} | \mathbf{v}_{k,\nu} \rangle_{\mathcal{T}}.
\]

The computational cost is \( \mathcal{O}(r_{u} r_{v} n d) \). The tensor rank can be truncated via the ALS-method or Gauss-Newton-method [35, 40]. The scalar product above helps to compute the Frobenius norm \( \| \mathbf{u} \|_{2} := \sqrt{\langle \mathbf{u} | \mathbf{v} \rangle_{\mathcal{T}}} \).

### 4.2 The Tensor Train format

The tensor train (TT) format is described in [97, 100, 59, 75]. As already noted, it was originally developed in quantum chemistry as “matrix product states” (MPS), see [118] and references therein, and rediscovered later [99, 100].
Definition 4.1 (TT-Format, TT-Representation, TT-Ranks). The TT-tensor format is for variable TT-representation ranks \( r = (r_0, \ldots, r_d) \in \mathbb{N}^{d+1} \) with \( r_0 = r_d = 1 \) and under the assumption that \( d > 2 \) — defined by the following multilinear mapping

\[
U_{TT} : P_{TT,r} := \prod_{\nu=1}^{d} P_{\nu}^{r_{\nu-1} \times r_{\nu}} \rightarrow T, \quad P_{\nu} = \mathbb{R}^{M_{\nu}} (\nu = 1, \ldots, d),
\]

\[
P_{TT,r} \ni P = (W^{(\nu)}) = (w^{(\nu)}_{j_1,j_2}) \in P_{\nu}^{r_{\nu-1} \times r_{\nu}} : 1 \leq j_{\nu} \leq r_{\nu}, 1 \leq \nu \leq d)
\]

\[
\mapsto U_{TT}(P) := w = \sum_{j_0=1}^{r_0} \cdots \sum_{j_d=1}^{r_d} \bigotimes_{\nu=1}^{d} w^{(\nu)}_{j_{\nu-1}j_{\nu}} \in T.
\]

We call \( w := (w_{i_1,\ldots,i_d}) = U_{TT,r}(P) \) a tensor represented in the train tensor format. Note that the TT-cores \( W^{(\nu)} \) may be viewed as a vector valued \( r_{\nu-1} \times r_{\nu} \) matrix with the vector \( w^{(\nu)}_{j_{\nu-1}j_{\nu}} \in \mathbb{R}^{M_{\nu}} \) with the components \( w^{(\nu)}_{j_{\nu-1}j_{\nu}}[i_{\nu}] : 1 \leq i_{\nu} \leq M_{\nu} \) at index position \( (j_{\nu-1}, j_{\nu}) \).

The representation in components is then

\[
(w_{i_1,\ldots,i_d}) = \sum_{j_0=1}^{r_0} \cdots \sum_{j_d=1}^{r_d} w^{(1)}_{j_{0}i_1} \cdots w^{(\nu)}_{j_{\nu-1}j_{\nu}}[i_{\nu}] \cdots w^{(d)}_{j_{d-1}j_{d}}[i_{d}]
\]

Equation (44)

Alternatively, each TT-core \( W^{(\nu)} \) may be seen as a vector of \( r_{\nu-1} \times r_{\nu} \) matrices \( W^{(\nu)}_{i_{\nu}} \) of length \( M_{\nu} \), i.e. \( W^{(\nu)} = (W^{(\nu)}_{i_{\nu}}) : 1 \leq i_{\nu} \leq M_{\nu} \). Then the representation Eq. (44) reads

\[
(w_{i_1,\ldots,i_d}) = \prod_{\nu=1}^{d} W^{(\nu)}_{i_{\nu}},
\]

which explains the name matrix product state. Observe that the first matrix is always a row vector as \( r_0 = 1 \), and the last matrix is always a column vector as \( r_d = 1 \). The matrix components \( W^{(\nu)}_{i_{\nu}} \) of the TT-cores are also called “carriages” or “waggons” with “wheels” \( i_{\nu} \) at the bottom, coupled to the next “carriage” or “wagon” via the matrix product. This explains the tensor train name. If one notes more carefully \( W^{(\nu)} \in P_{\nu}^{r_{\nu-1} \times r_{\nu}} = \mathbb{R}^{r_{\nu-1}} \otimes \mathbb{R}^{M_{\nu}} \otimes \mathbb{R}^{r_{\nu}} \), then Eq. (45) can be written more concisely as

\[
w = U_{TT}(P) = W^{(1)}_{1} \times_{3} W^{(2)}_{1} \times_{3} \cdots \times_{3} W^{(d)}_{1},
\]

Equation (46)

where \( U \times_{k} V \) is a contraction of the \( k \)-th index of \( U \) with the \( \ell \)-th index of \( V \), where one often writes just \( \times_{k} \) for \( \times_{k} \). Thus in Eq. (46) the contractions leave the indices from the \( \mathbb{R}^{M_{\nu}} \) untouched, so that the tensor \( w \) is formed.

Each TT-core (or block) \( W^{(\nu)} \) is defined by \( r_{\nu-1} \times r_{\nu} \times M_{\nu} \) numbers. Assuming \( n = M_{\nu} \) for all \( \nu = 1, \ldots, d \), the total number of entries scales as \( O(d n r^2) \), which is tractable as long as \( r = \max\{r_k\} \) is moderate.

We follow to the work of Oseledets [100] and list the major properties of the TT-tensor format.

The multiplication with scalar \( \alpha \) could be simply done by multiplying one of the TT-cores \( W^{(\nu)} \) in the representation Eq. (46) for any \( \nu \) in \( w = W^{(1)}_{1} \times_{3} W^{(2)}_{1} \times_{3} \cdots \times_{3} W^{(d)}_{1} \). But to balance the effect better, define \( \alpha_{\nu} := \sqrt{\nu} |\alpha| \) for all \( \nu > 1 \), and \( \alpha_1 := \text{sign}(\alpha) \sqrt{1} |\alpha| \). Then \( w = \alpha \cdot w \) is given by

\[
(\alpha_1 \cdot W^{(1)}_{1}) \times_{3} (\alpha_2 \cdot W^{(2)}_{1}) \times_{3} \cdots \times_{3} (\alpha_d \cdot W^{(d)}_{1}) = \tilde{W}^{(1)}_{1} \times_{3} \cdots \times_{3} \tilde{W}^{(d)}_{1}.
\]

The new cores are given by \( \tilde{W}^{(\nu)} = (\tilde{W}^{(\nu)}_{i_{\nu}}) = (\alpha_{\nu} W^{(\nu)}_{i_{\nu}}) \), a sequence of new “carriage” matrices. The computational complexity is \( O(d n r^2) \).
Addition of two TT-tensors Assume two tensors \( u \) and \( v \) are given in the TT-tensor format as in Eq. (45), i.e. \( (u_{i_1 \ldots i_d}) = \prod_{j=1}^d U_{i_j}^{(r)} \) and \( (v_{i_1 \ldots i_d}) = \prod_{j=1}^d \nu_{i_j}^{(e)} \). The sum \( w = u + v \) is given by the new cores \( W_{i_1 \ldots i_d}^{(\nu)} \) such that \( (w_{i_1 \ldots i_d}) = \prod_{j=1}^d W_{i_j}^{(\nu)} \), where

\[
W_{i_1}^{(\nu)} = \begin{pmatrix} U_{i_1}^{(\nu)} & 0 \\ 0 & V_{i_1}^{(\nu)} \end{pmatrix}, \quad 1 \leq i_\nu \leq r_\nu, 2 \leq \nu \leq d - 1.
\]

and the first and the last cores will be

\[
W_{1}^{(1)} = \begin{pmatrix} U_{1}^{(1)} \\ V_{1}^{(1)} \end{pmatrix} \quad \text{and} \quad W_{d}^{(d)} = \begin{pmatrix} U_{d}^{(d)} \\ V_{d}^{(d)} \end{pmatrix}.
\]

As only storage may have to be concatenated, the computational cost is \( O(1) \), but as the carriages resp. TT-cores grow, the final rank will generally be the sum of the ranks.

The Hadamard product \( w = u \odot v \) in the TT format is computed as follows. Assume two tensors \( u \) and \( v \) are given in the TT tensor format as in Eq. (45), i.e. \( (u_{i_1 \ldots i_d}) = \prod_{j=1}^d U_{i_j}^{(r)} \) and \( (v_{i_1 \ldots i_d}) = \prod_{j=1}^d \nu_{i_j}^{(e)} \). The Hadamard product is

\[
(w_{i_1 \ldots i_d}) = (u_{i_1 \ldots i_d} \cdot v_{i_1 \ldots i_d}).
\]

The tensor \( w \) has also the TT-tensor format, namely with the new cores

\[
W_{i_1 \ldots i_d}^{(\nu)} = U_{i_1}^{(\nu)} \otimes_K V_{i_1}^{(\nu)}, \quad 1 \leq i_\nu \leq r_\nu, 1 \leq \nu \leq d,
\]

where \( \otimes_K \) is the Kronecker product of two matrices [59]. The rank of \( W^{(\nu)} = (W_{i_1}^{(\nu)}) \) is the product of the ranks of the TT-cores \( U^{(\nu)} \) and \( V^{(\nu)} \).

The Euclidean inner product of two tensors in the TT-format as in Eq. (43)

\[
u = \sum_{j=1}^{r_1^u} \cdots \sum_{j_d=1}^{r_d^u} \otimes_{j=1}^d u_{j_1 \ldots j_d}^{(r)}, \quad v = \sum_{j=1}^{r_1^v} \cdots \sum_{j_d=1}^{r_d^v} \otimes_{j=1}^d v_{j_1 \ldots j_d}^{(e)},
\]

with ranks \( r^u \) and \( r^v \) can be computed as follows:

\[
\langle u \mid v \rangle_T = \sum_{j=1}^{r_1^u} \cdots \sum_{j_d=1}^{r_d^u} \sum_{i_1=1}^{r_1^v} \cdots \sum_{i_d=1}^{r_d^v} \prod_{j=1}^d \langle u_{j_1 \ldots j_d}^{(r)} \mid v_{j_1 \ldots j_d}^{(r)} \rangle_{p_{ij}}.
\]

The computational complexity is \( O(d n r^3) \), and can be reduced further [98].

Rank truncation in the TT format. The rank truncation operation is based on the SVD algorithm and requires \( O(d n r^3) \) operations [50]. The TT-rounding algorithm (p. 2305 in [100]) is based on QR decomposition and costs \( O(d n r^3) \).

Corollary 2.4 in [100] states that for a given tensor \( w \) and rank bounds \( r_k \), the best approximation to \( w \) in the Frobenius norm with TT-ranks bounded by \( r_k \) always exist (denote it by \( w^* \)), and the TT-approximation \( u \) computed by the TT-SVD algorithm (p. 2301 in [100]) is quasi-optimal:

\[
\| w - u \|_F \leq \sqrt{d - 1} \| w - w^* \|_F.
\]

(47)

In [79] the authors suggested a new re-compression randomised algorithm for Tucker and TT tensor formats. For the rank-adaptive DMRG-cross algorithm see [107], and its extension in [32].
5 Algorithms

As one may have gleaned from the preceding, very often not only the density \( p_\xi(y) \) is of interest, but expected values of functions of the density, e.g. in order to compute an \( f \)-divergence or the entropy. This section lists well-known numerical algorithms to actually compute functions from Table 3 like \( f(p_\xi(y)) \) by \( f(P) \), where the \( f \)'s considered are

\[
\{ \text{sign}(\cdot), (\cdot)^{-1}, \sqrt{\cdot}, \sqrt[\nu]{\cdot}, (\cdot)^k, \log(\cdot), \exp(\cdot), (\cdot)^2, |\cdot| \},
\]

where \( k > 0 \), and \( P \) is a tensor which represents the values of \( p_\xi(y) \) on a discretisation grid as explained in Subsection 2.3, i.e. \( P = p_\xi(\hat{X}) = \sum_{j=1}^{r_p} \otimes_{\nu=1}^d p_{j,\nu} \). The \( m \)-th root is needed for scaling.

Here we collect iterative algorithms and series expansions which have appeared in various places scattered in the literature, and which are used to compute functions in matrix algebras. As was shown in Section 2, these can also be used in the Hadamard algebra, which is isomorphic to an algebra of diagonal matrices. These algorithms are non-trivial and their detailed discussion is beyond the scope of this work, for this we point to the relevant literature. Specific possible difficulties which may appear if they are used in the low-rank representation are: the intermediate tensor ranks of iterates may become very large, or a stable rank truncation procedure may either not be available or it may be very computationally intensive. Included are also algorithms specific to low-rank tensor representations, the so-called cross-approximation, see Subsection 5.5.

5.1 Consistency of data

Making sure the data one works with is consistent is of great importance, and should be checked before any other computations. This was already touched upon at the end of Subsection 2.3. Recall that for the continuous case, the pdf has to be in the set \( \mathcal{D} \) (cf. Eq. (16)), and the pcf has to be in the set \( \mathcal{C} \) (cf. Eq. (19)). The discussion at the end of Subsection 2.3 also showed that these conditions are most easily checked by making sure that the discretised pdf (cf. Eq. (2)) is real valued and positive \( P \geq 0 \), and that the discrete integral Eq. (26) evaluates to unity, \( S(P) = 1 \).

That the pdf is real valued is translated by the Fourier transform (FT) into the pcf being Hermitean. The discrete FT preserves these properties, and these properties are preserved also in the low-rank representation. To check that the discretised low-rank representation of the pdf is real valued, one only has to make sure that the imaginary part vanishes—it does not even have to be represented.

The condition that the pdf is non-negative, which the Fourier transform (FT) translates into the pcf being positive definite, is preserved also by the discrete FT. But this is a local, point-wise condition, and it may be violated in the process of compression or low-rank approximation, and is also not so easily checked in a compressed low-rank format. It was already stated in Subsection 2.3 that this is equivalent to the positivity of the convolution operator \( K_\phi \) using the pcf tensor \( \Phi \), whose spectrum are the values of the pdf tensor \( P \), but this is not easily checked either. As will be shown later in Subsection 5.3, it is possible to compute the level set function \( \Lambda_U(P) \) Eq. (64) for the level set \( U = [0, \infty) \). In case this happens to be non-zero, indicating some indices \( i \) where \( P_i \geq 0 \) may be violated, one obtains a corrected pdf tensor \( P_c \) by setting

\[
P_c := P - \Lambda_U(P).
\]
This new approximation has all the faulty negative values removed, so that \( P_c \geq 0 \). This
change will not affect the Hermitean or self-adjoint character discussed earlier.

Through a correction like Eq. (49), or just due to the the process of compression or low-rank
approximation, the condition \( S(P) = 1 = \beta \) may not be satisfied any more. In case
this is not satisfied, say \( 1 \neq \beta > 0 \), for a re-scaled \( P_s \) one may set
\[
P_s := P/\beta.
\] (50)
This re-scaling will not affect the positive character of \( P \).

### 5.2 Overview of methods to compute tensor functions

The topic of point-wise functions was already discussed at the end of Subsection 2.3. There
are many methods to compute \( f(w) \). Most of these only use the fact that the underlying
structure (here of \( T \)) is that of a unital C*-algebra [109], and—at least implicitly—define the
functions via spectral calculus. Below we have collected and adapted some of the classical
matrix algorithms for computing the tensor functions listed above in Eq. (48).

Many algorithms developed (cf. [64]) to compute functions of matrices use only operations
from the underlying algebra. They can thus be used in any unital C*-algebra. Exponential
sums to compute \( w^{\circ-1} \) are implemented in [17, 13]. Some other methods and estimates
are developed in [49, 60, 71]. The function \( w^{\circ-1/2} \) was computed in [75, 71], and \( w^{\circ-\mu} \) in
[61, 71]. A quadrature rule to compute the Dunford-Cauchy contour integral for holomorphic
functions mentioned at the end of Subsection 2.3 is presented in [42, 43, 56, 57, 83, 75].
Iterative methods of Newton and Newton-Schultz type are used in [35, 40, 34, 11, 33]. The inversion \( w^{\circ-1} \) in the Tucker format is done by the Newton–Schultz approximate iteration in
[95].

The various TT-cross approximation algorithms [99, 7, 26, 25] are a well-known alternative
to iterative methods and series expansions, and they are sketched later in Subsection 5.5.
Whereas the previously mentioned algorithms work in any unital C*-algebra, the cross approx-
imation algorithms make use of a specific representation. We focus here on the tensor
train (TT) representation. The TT-cross approximation computes a low-rank TT approx-
imation of \( f(w) \) for a given function \( f(\cdot) \) and a tensor \( w \) directly, “on the fly”. The TT-cross
algorithms assume that the full tensor \( v := f(w) \) is not given explicitly, but rather as a
function which can return any element \( v_i := f(w_i) \) for a given index \( i \). The Tucker cross
algorithm to approximate \( w^{\circ-1} \) was used in [94]. In [116], the multigrid Cross 3D algorithm
is used to calculate the Gauss polynomial. In [96], iterative methods in the Tucker format
are used to compute \( w^{\circ1/3} \). In [7, 36], the authors are using the cross method for the Hier-
archical Tucker format to estimate various functionals of the solution in the UQ context. In
[63, 83] the sinc quadrature is used to compute fractional derivatives of the \( d \)-dimensional
Laplace operator. The TT-approximation of the sign function was computed in [24, 23], but
the TT-ranks were large. The point-wise inverse, level sets, and sign functions are defined
and computed in [33]. The point-wise inverse is required for computing the point-wise func-
tions \( \text{sign}(w) \) and \( \sqrt{w} \). [33]. The Newton algorithm for computing \( \text{sign}(w) \) and \( \exp(-w) \),
its convergence and error analysis for hierarchical matrices were considered in [52].

Polynomials are certainly the simplest functions, as they are directly elements of the
algebra. General polynomials one would numerically compute by e.g. using Horner’s scheme
in order to minimise the number of Hadamard products. Here only simple powers will be
needed as an auxiliary function for a kind of “scaling”, namely iterated squaring or iterated
inverse squaring. In some of the algorithms the scaling factor involves e.g. \( \|w\|_\infty \), we shall
sketch at the end of the following Subsection 5.3 how to compute that.
Denoting the power function by $w \mapsto w^m = \Psi_{\text{pow}}(m, w)$, one also wants to use it for negative powers; for $m < 0$ this is simply $\Psi_{\text{pow}}(m, w) = \Psi_{\text{pow}}(-m, w^{\ominus -1})$, and $w^{\ominus -1}$ is shown in Subsection 5.3. A really simple and well known way to make sure that no unnecessary multiplications are performed is for $m \in \mathbb{N}$ given by the recursive formula (although usually implemented in a loop):

$$\begin{align*}
\Psi_{\text{pow}}(m, w) = \begin{cases} 
  m > 1 \text{ and odd} : & w \odot \Psi_{\text{pow}}(m - 1, w); \\
  m \text{ even} : & \Psi_{\text{pow}}(m/2, w) \odot \Psi_{\text{pow}}(m/2, w); \\
  m = 1 : & w; 
\end{cases}
\end{align*}$$

(51)

Remark 5.1. While performing algebraic operations on tensors in some compressed format, the tensor ranks are increasing. To keep computational cost low, a tensor compression after each or after a number of algebraic operations may be necessary. We perform the truncation $T_\epsilon$ to low rank $r$ with error $\epsilon$ [59, 11]. We thus allow that the algebraic operations are possibly only executed approximately. It is assumed that such an approximation is performed whenever necessary, and it will not be always pointed out explicitly.

5.3 Iterative methods

We want to compute $f(w)$ for some function $f : T \rightarrow T$ from the list at the beginning of this section. We describe how to do it through iteration (see also [39]). Thus we have an iteration function $\Psi_f$, which only uses operations from the Hadamard algebra on $T$, and which is iterated, $v_{i+1} = \Psi_f(v_i)$, and converges to a fixed point $\Psi_f(v_*) = v_*$. When started with a $v_0$ depending on $w$, the fixed point is $\lim_{i \rightarrow \infty} v_i = v_* = \Psi_f(v_*) = f(w)$. A Newton-type family of high-order iterative methods for some matrix functions was discussed in [3].

To deal with truncation in iterative algorithms, the standard iteration map $\Psi_f$ is replaced by $T_\epsilon \circ \Psi_f$. Here one speaks about a perturbed or truncated iteration [62, 89, 39]. The general structure of the iterative algorithms for a post-processing task $f$ or for an auxiliary function is shown in Algorithm 1. In case the iteration by $\Psi_f$ is super-linearly convergent, the truncated iteration $T_\epsilon \circ \Psi_f$ will still converge super-linearly, but finally stagnate in an $\epsilon$-neighbourhood of the fixed point $v_*$. [62]. If the iteration by $\Psi_f$ is linearly convergent with contraction factor $q$, the truncated iteration $T_\epsilon \circ \Psi_f$ will still converge linearly, but finally stagnate in an $\epsilon/(1-q)$-neighbourhood of $v_*$. [89]. Ideas how to choose the starting value $v_0$ are given in [39].

Algorithm 1 Iteration with truncation

1: Input: tensor $v_0$; output: tensor $v_n$ after $n$ iterations
2: Start with some initial compressed guess $v_0 = w$.
3: $i \leftarrow 0$
4: while no convergence do
5: \hspace{1em} $v_{i+1} \leftarrow T_\epsilon \circ \Psi_f(v_i)$
6: \hspace{1em} $i \leftarrow i + 1$
7: end while

Computing the point-wise inverse $w^{\ominus -1}$. Apply Newton’s method to $F(x) := w - x^{\ominus -1}$ to approximate the inverse of a given tensor $w$, and one obtains [95] the following iteration
function $\Psi_{\odot^{-1}}$—to be used with Algorithm 1 with the initial iterate $v_0 = \alpha \cdot w$ to bring $v_0$ close to $v_n = 1$:

$$
\Psi_{\odot^{-1}}(v) = v \odot (2 \cdot 1 - w \odot v).
$$

(52)

The iteration converges if the initial iterate $v_0$ satisfies $\|1 - w \odot v_0\|_\infty < 1$. A possible candidate for the starting value is $v_0 = \alpha w$ with $\alpha < (1/\|w\|_\infty)^2$. For such a $v_0$, the convergence initial condition $\|1 - \alpha w^{-2}\|_\infty < 1$ is always satisfied. As the initial iterate was scaled, the fixed point of the iteration is $\nu_s = (1/\alpha) \cdot w^{\odot^{-1}}$, and thus the final result is $w^{\odot^{-1}} = \alpha \cdot \nu_s$.

We did not assume that $w$ is invertible, as the iteration actually computes the pseudo-inverse (i.e. only the non-zero entries are inverted). It is easily seen from Eq. (52) that with $v_0 = \alpha w$ zero entries in $w$ stay zero during the iteration.

**Computing point-wise $\sqrt{w}$ resp. $(w)_{\odot^{1/2}}$.** The Newton iteration for $F(x) := x^\odot 2 - w$ uses the iteration function Eq. (53) together with Algorithm 1.

$$
\Psi_{\sqrt{}}(v) = \frac{1}{2} \cdot (v + v^{\odot^{-1}} \odot w).
$$

(53)

The starting value can be $v_0 = (w + 1)/2$, other stating values obtained through scaling are described later. Unfortunately, Eq. (53) contains an inverse power $v^{\odot^{-1}}$ and can thus not be computed directly only with operations from the algebra. One could use the just described algorithm for the inverse, but the nested iteration is usually not so advantageous. An alternative is the well known stable inversion free Newton-Schulz iteration [64], which simultaneously computes $v^+ = w^{\odot^{1/2}}$ and its inverse $v^- = w^{\odot^{-1/2}}$. Setting $V_0 = [y_0, z_0] = [\alpha \cdot w, 1] \in \mathcal{T}^2$, the iteration function is best written using the auxiliary function $A(y, z) = 3 \cdot 1 - z \odot y$:

$$
\Psi_{\sqrt{}} \left( \begin{bmatrix} y \\ z \end{bmatrix} \right) = \frac{1}{2} \begin{bmatrix} y \odot A(y, z) \\ A(y, z) \odot z \end{bmatrix}.
$$

(54)

The iteration converges to $V_s = [v^+; v^-] = [\sqrt{y_0}, (\sqrt{y_0})^{\odot^{-1}}]$ if $\|1 - y_0\|_\infty < 1$, which can be achieved with a scaling factor $\alpha < 1/\|w\|_\infty$. As the initial iterate was scaled, the fixed point of the iteration is $v^+ = \sqrt{\alpha} \cdot \sqrt{w}$ and $v^- = (1/\sqrt{\alpha}) \cdot (\sqrt{w})^{\odot^{-1}}$. Thus the final result is $\sqrt{w} = (1/\sqrt{\alpha}) \cdot v^+$ and $(\sqrt{w})^{\odot^{-1}} = \sqrt{\alpha} \cdot v^-$. 

**Computing $w^{\odot^m}$ when $m \in \mathbb{N}$.** This function may be needed for logarithmic scaling purposes, see Subsection 5.4. For the theory and required definitions see Section 7 in [64]. A new family of high-order iterative methods for the matrix $m$-th root was suggested in [4]. To compute the principal $m$-th root of $w$, where it is assumed that $w \geq 0$, one considers Newton’s method for $F(x) = x^{\odot m} - w = 0$. The iteration function with $v_0 = w$ corresponding to Eq. (53) looks like

$$
\Psi_{m-\text{root}}(v) = \frac{1}{m} ((m - 1) \cdot v + \Psi_{\text{pow}}(1 - m, v) \odot v_0).
$$

(55)

If $m \geq 2$, this involves a negative power $v^{\odot(1-m)} = \psi_{\text{pow}}(1 - m, v)$. The convergence analysis is rather complicated, see more in Section 7.3, [64], but the algorithm converges for all $w \geq 0$. 

24
Just as there is a more stable version Eq. (54) for $m = 2$ avoiding inverses, so one has a “double iteration” [64] here as well. It is best written using the auxiliary function $A(y, z) = (1/m) \cdot ((m + 1) \cdot 1 - z)$:

$$
\psi_m \cdot \text{root} = \begin{bmatrix} y \\ z \end{bmatrix} = \begin{bmatrix} y \odot A(y, z) \\ \psi_{pow}(m, A(y, z)) \odot z \end{bmatrix},
$$

(56)

where $y_i \rightarrow w^{\odot \frac{1}{m}}$ and $z_i \rightarrow w^{\odot \frac{1}{m}}$. The starting values are $V_0 = [y_0, z_0] = [\alpha \cdot 1, (\alpha)^m w] \in \mathcal{T}^2$, with $\alpha < (\|w\|_\infty / \sqrt{2})^{-\frac{1}{m}}$. For scaling purposes it is best used with $m = 2^k$.

Another way of computing the $m$-th root is Tsai’s algorithm [113, 85], which uses the auxiliary function $B(y) = (2 \cdot 1 + (m - 2) \cdot y) \odot (1 + (m - 1) \cdot y)^{\odot -1}$:

$$
\psi_{\text{Tsa}} = \begin{bmatrix} y \\ z \end{bmatrix} = \begin{bmatrix} y \odot \psi_{pow}(m, B(y)) \\ z \odot (B(y)) \end{bmatrix},
$$

(57)

with starting value $V_0 = [w, 1]$. Then $z_i \rightarrow w^{\odot \frac{1}{m}}$.

**Computing sign($w$).** The tensor sign($w$) $\in \mathcal{T}$ is defined point-wise for all $i \in \mathcal{I}$ by

$$
\text{(sign($w$))}_i := \begin{cases} 
1, & w_i > 0; \\
-1, & w_i < 0; \\
0, & w_i = 0.
\end{cases}
$$

(58)

The equation to be used for the Newton iteration is $F(x) := x \odot x - 1$. With starting value $v_0 = w$ one obtains the following iteration function:

$$
\psi_{\text{sign}}(v) = \frac{1}{2}(\mu \cdot v + \frac{1}{\mu} \cdot v^{\odot -1}),
$$

(59)

with $\mu = \|v^{\odot -1}\|_\infty / \|v\|_\infty$ (cf. Section 8.6 in [64]). This method converges to sign($w$).

Alternatively, one can rewrite this iteration function without computing $v^{\odot -1}$, namely

$$
\psi_{\text{NS}}(v) = \frac{1}{2} \cdot v \odot (3 \cdot 1 - v \odot v),
$$

(60)

with starting value $v_0 = \alpha \cdot w$, where $\alpha = \|w^{\odot -1}\|_\infty / \|w\|_\infty$. The last formula is called the Newton-Schulz iteration, it has quadratic (local) convergence to sign($w$) [35, 33, 38, 64].

**Computing the absolute value |$w$|** is simple if sign($w$) Eq. (58) is available (see above): Having the sign($\cdot$) function, one can compute the absolute value, characteristic function of a set, and the level set function:

$$
|w| = w \odot \text{sign}(w).
$$

(61)

**Computing the characteristic function of a sub-set** of values $I \subset \mathbb{R}$ of a tensor $w$ can be done by using the shifted sign-function Eq. (58) [37, 38, 39]. The characteristic function of $w \in \mathcal{T}$ in an interval $I \subset \mathbb{R}$ is a tensor $\chi_I(w) \in \mathcal{T}$. It is defined for every multi-index $i$ point-wise as

$$
(\chi_I(w))_i := \begin{cases} 
1, & w_i \in I; \\
0, & w_i \notin I.
\end{cases}
$$

(62)

Let $a, b \in \mathbb{R}$. If $I = (-\infty, b)$, then $\chi_I(w) = \frac{1}{2}(1 + \text{sign}(b \cdot 1 - w))$. If $I = (a, +\infty)$, then $\chi_I(w) = \frac{1}{2}(1 - \text{sign}(a \cdot 1 - w))$. And if $I = [a, b]$, then

$$
\chi_I(w) = \frac{1}{2}(\text{sign}(b \cdot 1 - w) - \text{sign}(a \cdot 1 - w)).
$$

(63)
Computing the level set function of a sub-set of values $I \subset \mathbb{R}$ of a tensor $w$ may be accomplished using the characteristic function Eq. (63) [37, 38, 39]:

$$\Lambda_I(w) = \chi_I(w) \odot w.$$  \hspace{1cm} (64)

Computing $\|w\|_{\infty} = \max w = g(w)$ and $\min w$. We need these values in almost every algorithm above and for checking the consistency. For instance, if $\min w \geq 0$, then $w \geq 0$. It was already pointed out that $\|w\|_{\infty} = \max w = g(w)$ is the largest---by magnitude---eigenvalue of the associated linear operator $L_w : v \mapsto w \odot v$, and thus iterative eigenvalue algorithms can be used to compute it. One of the simplest is the power iteration. It can be modified in this special case here to greatly increase its convergence speed, essentially by repeated squaring. The modified power iteration algorithm is described in [53, 39]. The convergence is exponential with the rate $|\lambda_2/\lambda_1|^2$, where $\lambda_1$ and $\lambda_2$ are the largest and the second largest eigenvalues of $L_w$.

To compute $\min w$ (the smallest eigenvalue) or some intermediate eigenvalues of $L_w$ resp. $w$ we suggest to use the well-known shifting or inverse shifting functions [33, 39]. These and similar techniques are well known from eigenvalue calculations of large / sparse symmetric matrices [45, 102, 104, 119].

5.4 Series expansions

Computing $\log(w)$. We assume that $w > 0$. Various algorithms, improvement ideas, stability issues and tricks to compute $\log(w)$ are discussed in [20]. Improved inverse scaling and squaring algorithms for the matrix logarithm were suggested later in [2]. We suggest to follow these works for the case when $w$ is a tensor. The stability of the matrix arithmetic-geometric mean iterations for computing the matrix logarithm is investigated in [19]. For the algorithms to work well $w$ has to be close to the identity $\mathbf{1}$, which can be achieved by taking roots: for $\lambda > 0$ one has $\log(\lambda^k) = k \log \lambda$.

From matrix calculus it is known [20, 2] that one of the ways to compute $\log(w)$ for $w$ close to the identity is to truncate the Taylor series (radius of convergence $\|x\|_{\infty} < 1$):

$$\log(1 - x) = -\sum_{n=1}^{\infty} \frac{1}{n} \cdot x \odot^n$$

where $x := \mathbf{1} - w$. If $w$ is not near to the identity, then one may use the relation $\log(w) = 2^k \log(w \odot^{1/2^k})$, where $w \odot^{1/2^k} \to \mathbf{1}$ as $k$ increases [69].

Another way to compute the logarithm of a positive $w$ is Gregory’s series [64], which converges for all $w > 0$. Setting $z = (\mathbf{1} - w) \odot (\mathbf{1} + w)^{-1}$, one has

$$\log w = -2 \sum_{k=0}^{\infty} \frac{1}{2k + 1} \cdot z \odot^{2k+1}.$$  \hspace{1cm} (65)

Obviously, $z$ involves an inverse, but it has to be computed only once. We note that the tensor ranks (according to Section 4.2) in Eq. (65) may increase very fast.

Computing $\exp w$. One of the standard algorithms using power series together with scaling and squaring is explained in [64] (Chapter 10):

$$u_{r,s} = \left( \sum_{k=0}^{r} \frac{1}{k!s^k} w \odot^k \right)^{\odot s}.$$  \hspace{1cm} (66)
Here \( \lim_{r \to \infty} u_{r,s} = \lim_{s \to \infty} u_{r,s} = \exp w \). It is of advantage to use \( s \) from the series of powers of \( 2, s = 1, 2, 4, \ldots, 2^k \), then the \( s \)-th power can be computed by squaring. For the scaling the best choice is \( \alpha > \|w\|_\infty \).

### 5.5 Direct approximation by TT-cross-algorithms

In this section, we discuss the so-called cross algorithms \([99, 7, 26, 25]\) for \( v := f(w) \). Some extensions of the TT-Cross and ALS-Cross algorithms (e.g. the AMEn algorithm) were suggested by S. Dolgov and co-authors, and can be found in \([29]\).

A general cross algorithm computes the following TT-representation, see Subsection 4.2, the definition Eq. (43), and in particular Eq. (44):

\[
    f(w) = v(\alpha_1, \ldots, \alpha_M) = \sum_{s_1=1}^{r_1} \sum_{s_2=1}^{r_2} \cdots \sum_{s_{M-1}=1}^{r_{M-1}} v_{s_0,s_1}^{(1)}(\alpha_1) v_{s_1,s_2}^{(2)}(\alpha_2) \cdots v_{s_{M-1},s_M}^{(M)}(\alpha_M).
\]

(67)

For analytic \( f(\cdot) \) the TT-ranks often depend only logarithmically on the accuracy \([72, 108]\). These algorithms are an alternative to iterations and series expansions, they are tailored specifically to low-rank approximations in a particular tensor format. They allow one to compute a low-rank approximation of \( v = f(w) \) for a given function \( f(\cdot) \) and a tensor \( w \) directly, “on the fly”. We assume here that the full tensor \( v := f(w) \) is not given explicitly, but rather as a function which can return any element \( v_i := f(w_i) \) of \( v \).

For example, the AMEn algorithm can compute the representation Eq. (67) using only \( O(dnr^2) \) entries of \( v \) and \( O(dnr^3) \) additional arithmetic operations. The pseudocode is listed in \([25]\). It is based on the skeleton decomposition (another name is adaptive cross approximation) of a matrix \([47, 9, 8]\), and the maxvol algorithms \([46]\). The idea of the maxvol algorithms is to find a rank-\( r \) matrix approximation \( A_r \) of a \( n \times m \) matrix \( A \), the rank of which is \( r \). The maxvol algorithm suggests to select among all \( r \times r \) submatrices the one that has the largest volume (determinant). The computational complexity is \( O(r(n+m)) \), and the approximation error \( \|A - A_r\|_\infty \leq (r+1)\sigma_{r+1} \), where \( \sigma_{r+1} \) is the \( (r+1) \)-th singular value of \( A \).

### 6 Numerical examples

This section shows the real applicability of tensor techniques addressed in Sections 2–5. This includes a validation Example 6.1, where the KLD is computed with a well known analytical formula and the AMEn_cross algorithm \([32, 107]\) from the TT-toolbox for \( d \)-dimensional Gaussian pdfs. Further, in Example 6.2 the HELLinger distances are computed with the well known analytical formula as well as with the AMEn_cross algorithm. To show the approach on a distribution where the pdf is not known analytically, the \( d \)-variate elliptically contoured \( \alpha \)-stable distributions are chosen and accessed via their pdfs, and again KL and HELLinger distances for different value of \( d, n \), and the parameter \( \alpha \) are computed (Example 6.3).

For the numerical tests below we used the Matlab package TT-Toolbox \([100]\), which is well known in the tensor community. To compute \( f(w) \), we use the alternating optimization with enrichment (AMEn) method \([32]\), provided in the TT-toolbox library. This is a block cross algorithm with an error-based enrichment. It tries to interpolate the function \( f(w) \) via the error-enriched maxvol-cross method. All computations are done on a MacBook Pro computer produced in 2018, equipped with a 6-Core Intel Core i7 processor running at 2.2 GHz, and 16 GB RAM. We started by computing the point-wise inverse, squared root, and exponent of a given discretised pdf represented as a TT tensor. For this, iterative methods,
Table 4: $D_{KL}$ computed via TT tensors (AMEn algorithm) and the analytical formula Eq. (68) for various values of $d$. TT tolerance = $10^{-6}$, the stopping difference between consecutive iterations.

| $d$ | 16 | 32 | 64 |
|-----|----|----|----|
| $n$ | 2048 | 2048 | 2048 |
| $D_{KL}$ (exact) | 35.08 | 70.16 | 140.32 |
| $\bar{D}_{KL}$ | 35.08 | 70.16 | 140.32 |
| err$_a$ | 4.0e-7 | 2.43e-5 | 1.4e-5 |
| err$_r$ | 1.1e-8 | 3.46e-8 | 8.1e-8 |
| comp.time [s] | 1.0 | 5.0 | 18.7 |

series expansions, and the AMEn algorithm [32, 107] were used in order to make sure that the AMEn method gives the same results as other methods.

The first Example 6.1 is a validation example, where the analytical formula for the KLD is known analytically. This exact value is compared with the approximate KLD (denoted by $\bar{D}_{KL}$) for high values of $d$ and $n$. One may observe that they are almost the same. Additionally, the absolute error ($\text{err}_a := |D_{KL} - \bar{D}_{KL}|$) as well as the relative error ($\text{err}_r := |D_{KL} - \bar{D}_{KL}|/|D_{KL}|$) and the computing times (last row) are shown.

**Example 6.1 (Validation example 1 — KLD).** Consider two Gaussian distributions $\mathcal{N}_1 := \mathcal{N}(\mu_1, C_1)$ and $\mathcal{N}_2 := \mathcal{N}(\mu_2, C_2)$, where $C_1 := \sigma_1^2 I$, $C_2 := \sigma_2^2 I$, $\mu_1 = (1.1, \ldots, 1.1)$ and $\mu_2 = (1.4, \ldots, 1.4) \in \mathbb{R}^d$, $d = \{16, 32, 64\}$, $I$ is the identity matrix, and $\sigma_1 = 1.5$, $\sigma_2 = 22.1$. The well known analytical formula is [101]

$$D_{KL}(\mathcal{N}_1||\mathcal{N}_2) = \frac{1}{2} \left( \text{tr}(C_2^{-1}C_1) + (\mu_2 - \mu_1)^T C_2^{-1}(\mu_2 - \mu_1) - d + \log \left( \frac{|C_2|}{|C_1|} \right) \right).$$  (68)

After discretisation of the two pdfs, one obtains the tensors $P$ and $Q$ (cf. Section 1). Then the KLD $\bar{D}_{KL}$ is computed as in Table 2. The results are summarised in Table 4.

An important ingredient of the KLD computation is the $\log(\cdot)$ function, which can be computed via the AMEn method, or the Gregory series Eq. (65). We observed that the TT-ranks are increasing very fast in the Gregory series, and it is not so transparent how and when to truncate them. Therefore, we recommend using the AMEn algorithm (implemented in the TT Toolbox) for the approximation $\bar{D}_{KL}$ by computing on the fly the function $f(P, Q) = P \odot (\log(P) - \log(Q))$. The small absolute ($\text{err}_a$) and relative ($\text{err}_r$) errors show that the AMEn method can be used to compute the KLD.

The next validation test is with the Hellinger distance:

**Example 6.2 (Validation example 2 — Hellinger distance).** For the Gaussian distributions from Example 6.1, the Hellinger distances computed via the AMEn algorithm—denoted by $\bar{D}_H$ —and the analytical formula Eq. (69) denoted by $D_H$ are compared in Table 5. The squared Hellinger distances for two multi-variate Gaussian distributions can be computed analytically as follows (see p.51 and p.45 in [101]):

$$D_H(\mathcal{N}_1, \mathcal{N}_2)^2 = 1 - K_{1/2}(\mathcal{N}_1, \mathcal{N}_2), \quad \text{where} \quad$$

$$K_{1/2}(\mathcal{N}_1, \mathcal{N}_2) = \frac{\det(C_1)^{1/4} \det(C_2)^{1/4}}{\det(C_1 + C_2)^{1/2}} \cdot \exp \left( -\frac{1}{8}(\mu_1 - \mu_2)^T \left( \frac{C_1 + C_2}{2} \right)^{-1}(\mu_1 - \mu_2) \right).$$  (70)
Table 5: The Hellinger distance $D_H$ computed via TT tensors (AMEn algorithm) and the analytical formula Eq. (69) for various values of $d$. TT tolerance = $10^{-6}$. The Gaussian mean values and covariance matrices are defined in Example 6.1.

| $d$ | 16 | 32 | 64 |
|-----|----|----|----|
| $n$ | 2048 | 2048 | 2048 |
| $D_H$ (exact) | 0.99999 | 0.99999 | 0.99999 |
| $	ilde{D}_H$ | 0.99992 | 0.99999 | 0.99999 |
| err$_a$ | 3.5e-5 | 7.1e-5 | 1.4e-4 |
| err$_r$ | 2.5e-5 | 5.0e-5 | 1.0e-4 |
| comp.time [s] | 1.7 | 7.5 | 30.5 |

Table 6: Computation of $D_{KL}(\alpha_1, \alpha_2)$ for between two $\alpha$-stable distributions for $\alpha_1 = 2.0$, $\alpha_2 = 1.9$, and different $d$ and $n$. The AMEn tolerance is $10^{-9}$.

| $d$ | 16 | 16 | 16 | 16 | 16 | 16 | 32 | 32 | 32 |
|-----|----|----|----|----|----|----|----|----|----|
| $n$ | 8 | 16 | 32 | 64 | 128 | 256 | 64 | 128 | 256 |
| $D_{KL}(2.0, 1.9)$ | 0.016 | 0.059 | 0.06 | 0.062 | 0.06 | 0.09 | 0.14 | 0.12 |
| comp.time [s] | 0.8 | 3 | 8.9 | 14 | 22 | 61 | 207 | 80 | 78 |
| max. TT rank | 40 | 57 | 79 | 79 | 59 | 79 | 77 | 80 | 78 |
| memory, MB | 1.8 | 7 | 34 | 54 | 73 | 158 | 538 | 160 | 313 |

The results in Table 5 show that the AMEn algorithm is able to compute the $D_H$ Hellinger distance between two multivariate Gaussian distributions for large dimensions $d = \{16, 32, 64\}$, and for large $n = 2048$. The exact and approximate values are identical, and the error is small. The absolute and relative errors (err$_a$, err$_r$) can be further decreased by taking a smaller TT tolerance.

After these validation tests, we choose the $d$-variate elliptically contoured $\alpha$-stable distribution, where no analytical formula for the pdf is known, and which generalises the normal law. These distributions have heavy tails and are often used for modelling financial data [91]. We access the distribution in the next Example 6.3 through its pcf, which is known analytically Eq. (71).

**Example 6.3 ($\alpha$-stable distribution).** The pcf of a $d$-variate elliptically contoured $\alpha$-stable distribution is given by

$$
\varphi_\xi(t) = \exp \left( i \langle t \mid \mu \rangle - \langle t \mid C t \rangle^{\alpha/2} \right). \tag{71}
$$

We approximate $\varphi_\xi(t)$ as in Eq. (7), but in the TT format Eq. (43) and Eq. (67). The tolerance used in the AMEn algorithm is $10^{-9}$. Further, from the inversion theorem, the pdf of $\xi$ on $\mathbb{R}^d$ can be computed as in Eq. (8) via the FFT.

We start by computing the KLD between two $\alpha$-stable distributions for fixed $\alpha_1 = 2.0$, $\alpha_2 = 1.9$ (with $\mu_1 = \mu_2 = 0$, $C_1 = C_2 = I$); the results are summarised in Table 6.

From Table 6 one may see that $n = 32$ (for $d = 16$) is sufficient, and there is no need to take a higher resolution $n$, the KLD value is (almost) not changing. One may also see that for $d = 32$ one needs to take $n = 256$ or higher, but a higher $n$ requires more memory.
Table 7: Computation of $D_{KL}(\alpha_1, \alpha_2)$ between two $\alpha$-stable distributions for various $\alpha$ with fixed $d = 8$ and $n = 64$. AMEn tolerance is $10^{-12}$. $\mu_1 = \mu_2 = 0$, $C_1 = C_2 = I$.

| $(\alpha_1, \alpha_2)$ | (2.0, 0.5) | (2.0, 1.0) | (2.0, 1.5) | (2.0, 1.9) | (1.5, 1.4) | (1.0, 0.4) |
|------------------------|------------|------------|------------|------------|------------|------------|
| $D_{KL}(\alpha_1, \alpha_2)$ | 2.27       | 0.66       | 0.3        | 0.03       | 0.031      | 0.6        |
| comp.time [s]           | 8.4        | 7.8        | 7.5        | 8.5        | 11         | 8.7        |
| max. TT rank            | 78         | 74         | 76         | 76         | 80         | 79         |
| memory, MB              | 28.5       | 28.5       | 27.1       | 28.5       | 35         | 29.5       |

These values in the last column in Table 6, namely $d = 32$ and $n = 256$, can be used to illustrate the amount of data and computation which would be involved in a—here impossible—full representation. The values $d = 32$ and $n = 256$ mean that the amount of data in full storage mode would be $N = n^d = 265^{32} \approx 1.16E77$, and assuming 8 bytes per entry, this would be ca. $1E78$ bytes. Compare this to the estimated number of hadrons in the universe ($1E80$), to see that alone the storage of such an object is not possible in full mode, whereas in a TT-low-rank approximation it did not require more than ca. 626MB, and fits on a laptop. And as for the computation of the KLD shown in that table, assume that the computation of the logarithms per data point could be achieved at a rate of 1GHz. Then the KLD computation in full mode would require ca. $1.2E68$s, or more than $3E60$ years, and even with a perfect speed-up on a parallel super-computer with say 1,000,000 processors, this would require still more than $3E54$ years; compare this with the estimated age of the universe of ca. $1.4E10$ years.

Continuing our tests, in Table 7 the KLD $D_{KL}(\alpha_1, \alpha_2)$ between two $\alpha$-stable distributions for different pairs of $(\alpha_1, \alpha_2)$ and fixed $d = 8$ and $n = 64$ is computed. The mean and covariance matrices were taken $\mu_1 = \mu_2 = 0$, $C_1 = C_2 = I$. The tolerance for the AMEn algorithm was $10^{-12}$. These results demonstrate that a TT approximation is possible (although the TT ranks are not so small) for various values of the parameters $\alpha$ in Eq. (71).

From the KLD we turn again to the computation of the Hellinger distance, this time for the $d$-variate elliptically contoured $\alpha$-stable distribution. Table 8 shows the Hellinger distance $D_H(\alpha_1, \alpha_2)$ computed for two different $\alpha$-stable distributions with values of $\alpha = 1.5$ and $\alpha = 0.9$ for different $d$ and $n$. The mean values and the covariances are the same $\mu_1 = \mu_2 = 0$, $C_1 = C_2 = I$. The maximal TT ranks and the computation times are comparable to the KLD case in Table 6.

Table 8: Computation of $D_H(\alpha_1, \alpha_2)$ between two $\alpha$-stable distributions for different $d$ and $n$. AMEn tolerance is $10^{-9}$. $\mu_1 = \mu_2 = 0$, $C_1 = C_2 = I$.

| $d$   | 16 | 16 | 16 | 16 | 16 | 16 | 32 | 32 | 32 | 32 |
|-------|----|----|----|----|----|----|----|----|----|----|
| $n$   | 8  | 16 | 32 | 64 | 128| 256| 16 | 32 | 64 | 128|
| $D_H(1.5,0.9)$ | 0.218 | 0.223 | 0.223 | 0.223 | 0.219 | 0.223 | 0.180 | 0.176 | 0.175 | 0.176 |
| comp.time [s] | 2.8 | 3.7 | 7.5 | 19 | 53 | 156 | 11 | 21 | 62 | 117 |
| max. TT rank | 79 | 76 | 76 | 76 | 79 | 76 | 75 | 71 | 75 | 74 |
| memory, MB | 7.7 | 17 | 34 | 71 | 145 | 283 | 34 | 66 | 144 | 285 |
To show the influence of the TT (AMEn) tolerance, in Table 9 shows the $D_H$ distance computed with different TT (AMEn) tolerances. Additionally, the maximal tensor rank (there are $d$ ranks in total), the computing times, and the required storage cost are provided.

Table 9: Computation of $D_H(\alpha_1, \alpha_2)$ between two $\alpha$-stable distributions ($\alpha = 1.5$ and $\alpha = 0.9$) for different AMEn tolerances. $n = 128$, $d = 32$, $\mu_1 = \mu_2 = 0$, $C_1 = C_2 = I$.

| TT(AMEn) tolerance | $10^{-7}$ | $10^{-8}$ | $10^{-9}$ | $10^{-10}$ | $10^{-14}$ |
|---------------------|-----------|-----------|-----------|-----------|-----------|
| $D_H(1.5, 0.9)$     | 0.1645    | 0.1817    | 0.176     | 0.1761    | 0.1802    |
| comp. time [s]      | 43        | 86        | 103       | 118       | 241       |
| max. TT rank        | 64        | 75        | 75        | 78        | 77        |
| memory, MB          | 126       | 255       | 270       | 307       | 322       |

A note about software. Several tensor toolboxes developed for low-rank tensor calculus are available. The CP and Tucker decompositions are implemented in the Tensor Toolbox [5, 6, 1], and in the Tensorlab [117, 22]. The TT and QTT tensor formats are implemented in TT-toolbox [100]. The hierarchical Tucker tensor format is realised in the Hierarchical Tucker Toolbox [81]. For a more detailed overview, see [54, 76]. Almost all available implementations (e.g. TT-toolbox and htucker) have been used to solve (stochastic) PDEs [28], integral equations, linear systems in tensor format, or to perform arithmetic operations such as the scalar product, addition, etc. But, to the best of our knowledge, we do not know any attempts for computing the KLD and other divergences or distances, or the entropy of high-dimensional probability distributions. The Matlab files from our computations are freely available at https://github.com/litvinen/Divergence_in_tensors.git

7 Conclusion

The task considered here was the numerical computation of characterising statistics of high-dimensional pdfs, as well as their divergences and distances, where the pdf in the numerical implementation was assumed discretised on some regular grid. Even for moderate dimension $d$, the full storage and computation with such objects become very quickly infeasible.

We have demonstrated that high-dimensional pdfs, pcfs, and some functions of them can be approximated and represented in a low-rank tensor data format. Utilisation of low-rank tensor techniques helps to reduce the computational complexity and the storage cost from exponential $O(n^d)$ to linear in the dimension $d$, e.g. $O(dr^2)$ for the TT format. Here $n$ is the number of discretisation points in one direction, $r \ll n$ is the maximal tensor rank, and $d$ the problem dimension. The particular data format is rather unimportant, any of the well-known tensor formats (CP, Tucker, hierarchical Tucker, tensor-train (TT)) can be used, and we used the TT data format. Much of the presentation and in fact the central train of discussion and thought is actually independent of the actual representation.

In the beginning in Section 1 it was motivated through three possible ways how one may arrive at such a representation of the pdf. One was if the pdf was given in some approximate analytical form, e.g. like a function tensor product of lower-dimensional pdfs with a product measure, or from an analogous representation of the pcf and subsequent use of the Fourier transform, or from a low-rank functional representation of a high-dimensional RV, again via its pcf. The theoretical underpinnings of the relation between pdfs and pcfs as well as
their properties were recalled in Section 2, as they are important to be preserved in the discrete approximation. This also introduced the concepts of the convolution and of the point-wise multiplication Hadamard algebra, concepts which become especially important if one wants to characterise sums of independent RVs or mixture models, a topic we did not touch on for the sake of brevity but which follows very naturally from the developments here. Especially the Hadamard algebra is also important for the algorithms to compute various point-wise functions in the sparse formats. The Section 2, as well as the following Section 3 and Section 5 are actually completely independent of any particular discretisation and representation of the data.

Some statistics, divergences, and distance measures were collected in Section 3 together with the abstract discrete expressions on how to compute them numerically, independent of any particular numerical representation. To demonstrate our idea, one of the easiest tensor formats—the CP tensor format—was described first in Section 4. In the numerical part, we used the tensor-train (TT) format, which is also sketched in Section 4, together with how to implement the operations of the Hadamard algebra. As Section 3 shows, point-wise functions are required in order to compute the desired statistics, and some algorithms to actually perform this in an algebra were collected in Section 5. These were originally developed for matrix algebra algorithms [64], but they work just as well in any other associative C∗-algebra. In using such algorithms, one assumes that the ranks of the involved tensors are not increasing strongly during iterations and linear algebra operations.

In the numerical computations in Section 6, the first example is one where the analytic answer was known, and this validates the approach and shows the accuracy of the low-rank computation in the computation of KL and Hellinger distances, which were taken as examples of characterising functionals resp. statistics. As a more taxing problem, we then took elliptically contoured α-stable distributions to evaluate the KLD and Hellinger distances between them. For these distributions, the pdf is not known analytically, but the pcf is, which we took as our starting point. The AMEn TT-Cross algorithm [24, 25] was used to compute the low-rank approximations, and the pdfs were then computed via FFT. This also nicely demonstrates the smooth integration of the FFT into low-rank tensor formats, and made it subsequently possible to compute the required quantities.

In total, these examples showed the viability of this concept, namely that it is possible to numerically operate on discretised versions of high-dimensional distributions with a reasonable computational expense, whereas in a full format the computations would not have been feasible at all. All that we required was that the data in its discretised form can be considered as an element of a commutative C∗-algebra with an inner product, where the algebra operations only have to be numerically computed in an approximative fashion. Such an algebra is isomorphic to a commutative sub-algebra of the usual matrix algebra, allowing the use of matrix algorithms.

Acknowledgments

The research reported in this publication was partly supported by funding from the Alexander von Humboldt Foundation (AvH), the Deutsche Forschungsgemeinschaft (DFG), and a Gay-Lussac Humboldt Prize. We also would like to thank Sergey Dolgov (University of Bath, UK) for his assistance with the TT-toolbox.
References

[1] E. Acar, D. M. Dunlavy, and T. G. Kolda, *A scalable optimization approach for fitting canonical tensor decompositions*, J Chemom. 25 (2011), no. 2, 67–86, doi:10.1002/cem.1335.

[2] A. H. Al-Mohy and N. J. Higham, *Improved inverse scaling and squaring algorithms for the matrix logarithm*, SISC 34 (2012), no. 4, C153–C169, doi:10.1137/110852553.

[3] S. Amat, S. Busquier, and A. A. Magrenan, *On a Newton-type family of high-order iterative methods for some matrix functions*, AIP Conf. Proc. 1978 (2018), no. 1, 330005, doi:10.1063/1.5043941.

[4] S. Amat, J. A. Ezquerro, and M. A. Hernandez-Veron, *On a new family of high-order iterative methods for the matrix p-th root*, Numer. Linear Algebra Appl. 22 (2015), no. 4, 585–595, doi:10.1002/nla.1974.

[5] B. W. Bader and T. G. Kolda, *Algorithm 862: MATLAB tensor classes for fast algorithm prototyping*, ACM Trans. Math. Softw. 32 (2006), no. 4, 635–653, doi:10.1145/1186785.1186794.

[6] B. W. Bader, T. G. Kolda, et al., *Matlab tensor toolbox version 2.6*, Available online, February 2015, Available from: http://www.sandia.gov/~tgkolda/TensorToolbox/.

[7] J. Ballani and L. Grasedyck, *Hierarchical tensor approximation of output quantities of parameter-dependent PDEs*, SIAM-ASA J Uncertain 3 (2015), 852–872, doi:10.1137/140960980.

[8] M. Bebendorf, *Adaptive cross approximation of multivariate functions*, Constr. Approx. 34 (2011), no. 2, 149–179, doi:10.1007/s00365-010-9103-x.

[9] M. Bebendorf and S. Rjasanow, *Adaptive low-rank approximation of collocation matrices*, Computing 70 (2003), no. 1, 1–24. MR MR1972724 (2004a:65177).

[10] D. Belomestny and L. Iosipoi, *Fourier transform MCMC, heavy-tailed distributions, and geometric ergodicity*, Math. Comput. Simul. 181 (2021), 351–363, doi:10.1016/j.matcom.2020.10.005.

[11] U. Benedikt, H. Auer, M. Espig, W. Hackbusch, and A. A. Auer, *Tensor representation techniques in post-Hartree–Fock methods: matrix product state tensor format*, Molecular Physics 111 (2013), no. 16–17, 2398–2413, doi:10.1080/00268976.2013.798433.

[12] P. Benner, M. Ohlberger, A. Cohen, and K. Willcox, *Model reduction and approximation*, Society for Industrial and Applied Mathematics, Philadelphia, PA, 2017, doi:10.1137/1.9781611974829.

[13] G. Beylkin and L. Monzon, *On approximation of functions by exponential sums*, Appl. Comput. Harmon. Anal. 19 (2005), 17–48, doi:10.1016/j.acha.2005.01.003.

[14] J. Biamonte and V. Bergholm, *Quantum tensor networks in a nutshell [online], arXiv: 1708.00006 [quant-ph], July 2017*, Available from: https://arxiv.org/abs/1708.00006, arXiv:1708.00006.

[15] D. Bigoni, A. P. Engsig-Karup, and Y. M. Marzouk, *Spectral tensor-train decomposition*, SISC 38 (2016), no. 4, A2405–A2439, doi:10.1137/15M1036919.

[16] R. N. Bracewell, *The Fourier transform and its applications*, McGraw-Hill, New York, NY, 1978.

[17] D. Braess and W. Hackbusch, *Approximation of 1/x by exponential sums in [1,∞],IMA J. Numer. Anal. 25 (2005), 685–697, doi:10.1093/imanum/dri015.

[18] J. C. Bridgeman and C. T. Chubb, *Hand-waving and interpretive dance: An introductory course on tensor networks*, J. Phys. A: Math. Theor. 50 (2017), 223001, doi:10.1088/1751-8121/aa5dc3.

[19] J. R. Cardoso and R. Ralha, *Matrix arithmetic-geometric mean and the computation of the logarithm*, SIAM J. Matrix Anal. Appl. 37 (2016), no. 2, 719–743, doi:10.1137/140998226.

[20] S. H. Cheng, N. J. Higham, C. S. Kenney, and A. J. Laub, *Approximating the logarithm of a matrix to specified accuracy*, SIAM J. Matrix Anal. Appl. 22 (2001), no. 4, 1112–1125, doi:10.1137/S0895479899364015.

[21] A. Cichocki and S. Amari, *Adaptive blind signal and image processing: Learning algorithms and applications*, Wiley, 2002.

[22] L. De Lathauwer, B. De Moor, and J. Vandewalle, *A multilinear singular value decomposition*, SIAM J. Matrix Anal. Appl. 21 (2000), 1253–1278.
[23] S. Dolgov, B. N. Khoromskij, A. Litvinenko, and H. G. Matthies, Computation of the response surface in the tensor train data format [online], arXiv: 1406.2816 [math.NA], Available from: https://arxiv.org/abs/1406.2816.

[24] S. Dolgov, B. N. Khoromskij, A. Litvinenko, and H. G. Matthies, Polynomial chaos expansion of random coefficients and the solution of stochastic partial differential equations in the tensor train format, SIAM-ASA J. Uncertain. 3 (2015), no. 1, 1109–1135.

[25] S. Dolgov, A. Litvinenko, and D. Liu, Kriging in tensor train data format, Proceedings, 3rd Int. Conf. on Uncert. Quantif. in CSE, 2019, pp. 309–329, Available from: https://files.eccomasproceedia.org/papers/e-books/uncecompp_2019.pdf, doi:10.7712/120219.6343.18651.

[26] S. Dolgov and R. Scheichl, A hybrid Alternating Least Squares - TT Cross algorithm for parametric PDEs [online], arXiv: 1707.04562 [math.NA], 2017, Available from: https://arxiv.org/abs/1707.04562.

[27] S. Dolgov, B. N. Khoromskij, and D. V. Savostyanov, Superfast Fourier transform using QTT approximation, J. Chem. Phys. 18 (2012), no. 5, 915–953.

[28] S. Dolgov, Additional UQ and statistical procedures for TT-toolbox, 2021, Available from: https://people.bath.ac.uk/sd901/research/software/.

[29] ______, Tensor Train ALS-cross algorithm and experiments, 2021, Available from: https://people.bath.ac.uk/sd901/als-cross-algorithm/.

[30] S. Dolgov, K. Anaya-Izquierdo, C. Fox, and R. Scheichl, Approximation and sampling of multivariate probability distributions in the tensor train decomposition, Statistics and Computing 30 (2020), no. 3, 603–625, doi:10.1007/s11222-019-09910-z.

[31] S. Dolgov, D. Kressner, and C. Strössner, Functional Tucker approximation using Chebyshev interpolation [online], arXiv: 2007.16126 [math.NA], 2020, Available from: https://arxiv.org/abs/2007.16126.

[32] S. Dolgov and D. Savostyanov, Alternating minimal energy methods for linear systems in higher dimensions, SISC 36 (2014), no. 5, A2248–A2271 (English), doi:10.1137/140953289.

[33] M. Espig, W. Hackbusch, A. Litvinenko, H. G. Matthies, and E. Zander, Efficient analysis of high dimensional data in tensor formats, Sparse Grids and Applications (J. Garcke and M. Griebel, eds.), Lecture Notes in Computational Science and Engineering, vol. 88, Springer, Berlin, 2013, pp. 31–56 (English), doi:10.1007/978-3-642-31703-3_2.

[34] M. Espig, W. Hackbusch, S. Handschuh, and R. Schneider, Optimization problems in contracted tensor networks, Comput. Vis. Sci. 14 (2011), no. 6, 271–285, doi:10.1007/s00304-012-0159-0.

[35] M. Espig, Efficient Bestapproximation mittels Summen von Elementartensobern in hohen Dimensionen, Ph.D. thesis, Universität Leipzig, Germany, 2008.

[36] M. Espig, L. Grasedyck, and W. Hackbusch, Black box low tensor-rank approximation using fiber-crosses, Constr. Approx. 30 (2009), 557–597, doi:10.1007/s00365-009-9076-9.

[37] M. Espig and W. Hackbusch, A regularized Newton method for the efficient approximation of tensors represented in the canonical tensor format, Numer. Math. 122 (2012), no. 3, 489–525, doi:10.1007/s00211-012-0465-9.

[38] M. Espig, W. Hackbusch, S. Handschuh, and R. Schneider, Optimization problems in contracted tensor networks, Comput. Vis. Sci. 14 (2011), no. 6, 271–285, doi:10.1007/s00304-012-0183-y.

[39] M. Espig, W. Hackbusch, A. Litvinenko, H. G. Matthies, and E. Zander, Iterative algorithms for the post-processing of high-dimensional data, J. Comput. Phys. 410 (2020), 109396, doi:10.1016/j.jcp.2020.109396.

[40] M. Espig, W. Hackbusch, T. Rohwedder, and R. Schneider, Variational calculus with sums of elementary tensors of fixed rank, Numer. Math. 122 (2012), no. 3, 469–488, doi:10.1007/s00211-012-0464-x.

[41] G. Evenbly and G. Vidal, Tensor network states and geometry, J Stat Phys 145 (2011), 891–918, doi:10.1007/s10955-011-0237-4.
[84] M. Loève, Probability theory I. graduate texts in mathematics, vol. 45, 46., fourth ed., Springer, Berlin, 1977. MR MR0651017 (58 #31324a)
[85] E. Lorin and S. Tian, A numerical study of fractional linear algebraic systems, Math. Comput. Simul. 182 (2021), 495–513, doi:10.1016/j.matcom.2020.11.010.
[86] E. Lukacs, Characteristic Functions, Griffin, London, 1970.
[87] H. G. Matthies and A. Keese, Galerkin methods for linear and nonlinear elliptic stochastic partial differential equations, Comput. Methods Appl. Mech. Engrg. 194 (2005), no. 12–16, 1295–1331, doi:10.1016/j.cma.2004.05.027. MR MR2121216 (2005j:65146)
[88] H. G. Matthies, Uncertainty quantification with stochastic finite elements, Encyclopedia of Computational Mechanics (E. Stein, R. de Borst, and T. J. R. Hughes, eds.), vol. 1, Wiley, 2007, doi:10.1002/0470091355.ecm071.
[89] H. G. Matthies and E. Zander, Solving stochastic systems with low-rank tensor compression, Linear Algebra Its Appl. 436 (2012), 3819–3838, doi:10.1016/j.laa.2011.04.017.
[90] F. Nielsen and R. Nock, On the Chi square and higher-order Chi distances for approximating f-divergences [online], arXiv: 1309.3029 [cs.IT], 2013, Available from: https://arxiv.org/abs/1309.3029, arXiv:1309.3029.
[91] J. P. Nolan, Multivariate elliptically contoured stable distributions: theory and estimation, Comput. Stat. 28 (2013), no. 5, 2067–2089, doi:10.1007/s00180–013–0396–7.
[92] W. Nowak and A. Litvinenko, Kriging and spatial design accelerated by orders of magnitude: Combining low-rank covariance approximations with FFT-techniques, Mathematical Geosciences 45 (2013), no. 4, 411–435, doi:10.1007/s11004–013–9453–6.
[93] R. Orú, A practical introduction to tensor networks: Matríz product states and projected entangled pair states, Annals of Physics 349 (2014), 117–158, doi:10.1016/j.aop.2014.06.013.
[94] I. Oseledets, D. Savostianov, and E. Tyrtyshnikov, Tucker dimensionality reduction of three-dimensional arrays in linear time, SIAM J. Matrix Anal. Appl. 30 (2008), no. 3, 939–956, doi:10.1137/060655894.
[95] I. V. Oseledets, D. V. Savostyanov, and E. E. Tyrtyshnikov, Linear algebra for tensor problems, Computing 85 (2009), no. 3, 169–188, doi:10.1007/s00607–009–0047–6.
[96] I. Oseledets and E. Tyrtyshnikov, TT-cross approximation for multidimensional arrays, Linear Algebra Appl. 432 (2010), no. 6, 935–952, doi:10.1016/j.laa.2009.07.024.
[97] I. Oseledets and E. Tyrtyshnikov, Breaking the curse of dimensionality, or how to use SVD in many dimensions, SISC 31 (2009), no. 5, 3744–3759.
[98] I. Oseledets, Matlab TT-toolbox, version 2.2, 2011, Available from: http://spring.imm.ras.ru/oseel/?page_id=24.
[99] I. Oseledets and E. Tyrtyshnikov, TT-cross approximation for multidimensional arrays, Linear Algebra Appl. 432 (2010), 70–88, doi:10.1016/j.laa.2009.07.024.
[100] I. V. Oseledets, Tensor-train decomposition, SIAM J. Sci. Comput. 33 (2011), no. 5, 2295–2317, Software https://github.com/oseledets/TT-Toolbox.git, doi:10.1137/090752286.
[101] L. Pardo, Statistical inference based on divergence measures, CRC press, 2018.
[102] B. N. Parlett, The symmetric eigenvalue problem, SIAM, Philadelphia, PA, 1998.
[103] P. B. Rohrbach, S. Dolgov, L. Grasedyck, and R. Scheichl, Rank Bounds for Approximating Gaussian Densities in the Tensor-Train Format [online], arXiv:2001.08187 [math.NA], 2020, Available from: https://arxiv.org/abs/2001.08187, arXiv:2001.08187.
[104] Y. Saad, Numerical methods for large eigenvalue problems: Theory and algorithms, Manchester University Press, Manchester, 1992.
[105] S. Sachdev, Tensor networks—a new tool for old problems, Physics 2 (2009), 90, doi:10.1103/Physics.2.90.
[106] Z. Sasvari, Multivariate characteristic and correlation functions, vol. 50, De Gruyter, 2013.
[107] D. V. Savostyanov and I. V. Oseledets, *Fast adaptive interpolation of multi-dimensional arrays in tensor train format*, Proceedings of 7th International Workshop on Multidimensional Systems (nDS), IEEE, 2011, doi:10.1109/nDS.2011.6076873.

[108] R. Schneider and A. Uschmajew, *Approximation rates for the hierarchical tensor format in periodic sobolev spaces*, Journal of Complexity 30 (2014), no. 2, 56–71, doi:10.1016/j.jco.2013.10.001.

[109] I. E. Segal and R. A. Kunze, *Integrals and Operators*, Springer, Berlin, 1978.

[110] N. Shephard, *From characteristic function to distribution function: a simple framework for the theory*, Econometric Theory 7 (1991), 519–529.

[111] A. Smilde, R. Bro, and P. Geladi, *Multi-way analysis with applications in the chemical sciences*, Wiley, 2004.

[112] T. L. Toulias and C. P. Kitsos, *Information divergence and the generalized normal distribution: A study on symmetricity*, Commun. Math. Stat. (2020), doi:10.1007/s40304-019-00200-8.

[113] J. S. H. Tsai, L. S. Shieh, and R. E. Yates, *Fast and stable methods for computing the principal nth root of a complex matrix and the matrix sector function*, Comput. Math. Appl. 15 (1988), no. 11, 903–913, doi:10.1016/0898-1221(88)90034-x.

[114] L. R. Tucker, *Some mathematical notes on three-mode factor analysis*, Psychometrika 31 (1966), 279–311.

[115] M. Udell and A. Townsend, *Why are big data matrices approximately low rank?*, SIMODS 1 (2019), no. 1, 144–160, doi:10.1137/18M1183480.

[116] D. V. Savostyanov, E. Tyrtyshnikov, B. Khoromskij, and H.-J. Flad, *Verification of the cross 3d algorithm on quantum chemistry data*, Russian J. Numer. Anal. Math. Modelling 23 (2008), 329–344, doi:10.1515/RJNAMM.2008.020.

[117] N. Vervliet, O. Debals, L. Sorber, M. Van Barel, and L. De Lathauwer, *Tensorlab 3.0*, online, 2016, Available from: http://www.tensorlab.net.

[118] G. Vidal, *Efficient classical simulation of slightly entangled quantum computations*, Phys. Rev. Lett. 91 (2003), 147902, doi:10.1103/PhysRevLett.91.147902.

[119] D. Watkins, *The matrix eigenvalue problem: GR and Krylov subspace methods*, SIAM, Philadelphia, PA, 2007.

[120] V. Witkovsky, *Numerical inversion of a characteristic function: An alternative tool to form the probability distribution of output quantity in linear measurement models*, ACTA IMEKO 5 (2016), no. 3, 32–44.

[121] V. Witkovsky, G. Wimmer, and T. Duby, *Computing the aggregate loss distribution based on numerical inversion of the compound empirical characteristic function of frequency and severity*, arXiv preprint:1701.08299, 2017, Available from: http://arxiv.org/abs/1701.08299.
