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Tensor approximation of stationary distributions of chemical reaction networks*

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Abstract

We prove that the stationary distribution of a system of reacting species with a weakly-reversible reaction network of zero deficiency in the sense of Feinberg admits tensor-structured approximation of complexity which scales linearly with respect to the number of species and logarithmically in the maximum copy numbers as well as in the desired accuracy. Our results cover the classical mass-action and also Michaelis–Menten kinetics which correspond to two widely used classes of propensity functions, and also to arbitrary combinations of those. New rank bounds for tensor-structured approximations of the PDF of a truncated one-dimensional Poisson distribution are an auxiliary result of the present paper, which might be of independent interest.

The present work complements recent results obtained by the authors jointly with M. Khammash and M. Nip on the tensor-structured numerical simulation of the evolution of system states distributions, driven by the Kolmogorov forward equation of the system, known also as the *chemical master equation*, or CME for short. For the two kinetics mentioned above we also analyze the low-rank tensor structure of the CME operator.

Keywords: chemical master equation, stochastic models, low rank, tensor approximation, tensor train, quantized tensor train, multilinear algebra, mass-action kinetics, Michaelis–Menten kinetics, stationary distribution, deficiency zero, chemical reaction network, Poisson distribution .

AMS Subject Classification (2000): 15A69, 34K21, 34K28, 41A25, 60J27, 92C42.

1 Introduction

In recent years, there has been an increasing awareness that large classes of mathematical models which arise in the description of physical phenomena with multiple scales, with continuum-atomistic coupling and with complex systems involve differential equations on high- and possibly infinite-dimensional state- and parameter spaces. Accordingly, discretization methods for the efficient numerical solution of such differential equations have received increasing attention. Among these methods, we mention only sparse grids, Smolyak interpolation and quadrature and hyperbolic cross approximation. In computational chemistry, for several decades now *tensor structured numerical computations* have been successfully used for the efficient numerical approximation of high-dimensional electron structure computations.

Another class of high-dimensional problems of similarly fundamental importance in life- and biological system sciences is the *chemical master equation* (CME for short). This equation describes the statistical behaviour of species in chemical reactions. The statistical behaviour is represented via the corresponding *probability density function* (PDF) which, analogous to the electron density in quantum-mechanical descriptions of electron structure in chemistry, is a

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deterministic function of many variables; specifically, of as many variables as there are chemical species in the system.

Due to its central significance for the modelling and the quantitative understanding of basic processes in life-sciences (see, for instance, [1, 2]), the efficient numerical solution of the CME has received substantial attention in recent years. Due to the high-dimensionality, stochastic methods have been widely used (see, e.g., [3, 4]). Deterministic numerical solution approaches which attempt the direct solution of the Kolmogorov equation have been so far limited to systems with a moderate number of species; see, for example, [5, 6, 7, 8, 9] and the references there. One key problem, the possibly infinite size of the state-space, has been handled with what is now called *Finite State Projection* (FSP for short); see [10, 11].

Very recently, in [12, 13, 14] the use of tensor structured numerical linear algebra methods has been proposed to avoid the excessive use of memory and the unfavourable scaling of computational complexity with respect to the number of species and maximum copy numbers, which arises in standard numerical methods for the solution of the CME. In these references, tensor structured solvers which rely on the adaptive low-rank representation of state vectors at each step of the calculation were implemented for the numerical solution of the CME. In numerical experiments, these methods were found in [13, 14] to perform superior to known deterministic and stochastic approaches, in terms of CPU and memory scaling vs. accuracy. This observed good performance of tensor-structured numerical methods in particular examples motivates further theoretical analysis of these methods in the context of the CME.

One question of particular interest in connection with these simulations is that of existence and computation of *invariant distributions* of the probability density; in the numerical experiments in [13, 14] it was observed in several benchmark examples that the time-evolution of the probability density function of several basic systems "settles" exponentially fast, after a transient phase where the efficient storage requires high tensor ranks for tracking the evolution of the probability density accurately, on a stationary solution. This solution, as a rule, turns out to admit the representation in terms of rather few parameters, even for systems with a large number of species.

To justify this empirical observation mathematically, at least for particular classes of systems, is the purpose of the present paper. Specifically, we show here that for Chemical Reaction Networks (CRNs for short) with deficiency zero in the sense of Feinberg [15, 16, 17] and for a certain class of propensity functions that the stationary PDF of such systems allows for approximation of accuracy $\varepsilon > 0$ with tensor ranks r which scale logarithmically in the accuracy as well as in the maximum copy numbers, and which are linearly scaling in the number of chemical species present in the system.

The outline of this paper is as follows. In Section 2 we recapitulate basic definitions and notations from the theory of chemical reaction networks, and present in particular the basic result of Anderson et al. [16] on the stationary distribution of the CME describing such systems.

In Section 2 we recapitulate the notion of *chemical reaction networks* and summarize the deficiency zero theory of Feinberg [15, 18, 19, 20]. Also, we present the recent result of [16] on the relation between the stochastic and deterministic models, which serves as a starting point for our analysis. Finally, we outline the *finite state projection* approach of Munsky and Khammash [10, 11] for the approximation of the dynamics of the CME to finitely many states.

In Section 3.1, we revisit briefly the basic concepts of the *tensor train (TT)* representation of multidimensional arrays due to Oseledets and Tyrtyshnikov, and its extension to the so-called *quantized tensor train* (*QTT* for short) format proposed by Oseledets in [21, 22] and by Khoromskij in [23]. In particular, Section 3.3 collects preliminary results, some cited and new, which underlie the main results of the present paper.

In Section 4, we give rank bounds for the QTT-structured representation of the CME operator; we develop these bounds under the general assumption that the propensity functions are separable and that the factors in these representations admit QTT-structured approximations with low ranks. We recapitulate the result of [14] on the structure on the corresponding approximation of the CME operator and extend it by quantifying the associated error.

Section 5 presents our main results. In particular, the QTT structure of the factors of separable stationary distributions for weakly reversible chemical reaction networks of zero deficiency in the sense of Feinberg. Finally, we show error bounds which are implied by those for QTT structured approximation of the stationary distribution itself. The QTT structure of the PDF of a truncated one-dimensional Poisson distribution (Theorem 22) is an auxiliary result of this section.

2 Chemical reaction networks

2.1 Terminology

Consider a system of d reacting chemical *species* $\mathcal{S} = \{S_1, \ldots, S_d\}$ collected symbolically into the vector $S = (S_1, S_2, ..., S_d)^\top$. Define $\mathcal{Z} = \mathbb{Z}^d_{\geq 0}$ and for all $\nu_s, \nu'_s \in \mathcal{Z}$ denote symbolically ${\nu_s}^\top S = \nu_{s1}S_1 + \ldots + \nu_{sd}S_d$ and ${\nu'_s}^\top S = \nu'_{s1}S_1 + \ldots + \nu'_{sd}S_d$. Then, if the chemical *reaction* ${\nu_s}^\top S \to {\nu'_s}^\top S$ can occur in the system, the vectors ν_s and ν'_s, identified with the combinations ${\nu_s}^\top S$ and ${\nu'_s}^\top S$ of species, represent the chemical *source* and *product complexes* consumed and produced in the reaction, respectively. The difference $\eta_s = \nu'_s - \nu_s \in \mathbb{Z}^d$ indicates the change in the copy numbers of all components caused by the reaction and is called the *stoichiometry vector* of the reaction. We consider a system with R reactions indexed by s varying from 1 to R, each reaction being given through the corresponding complexes $\nu_s, \nu'_s \in \mathcal{Z}$. We denote with $\mathcal{C} = \{\nu_s, \nu'_s\}_{s=1}^R$ the set of all complexes; and by $\mathcal{R} = \{(\nu_s \to \nu'_s)\}_{s=1}^R$, the set of all reactions.

Definition 1. *The triple* $\{\mathcal{S}, \mathcal{C}, \mathcal{R}\}$ *is called a* chemical reaction network*, or* CRN *for short.*

A CRN $\{\mathcal{S}, \mathcal{C}, \mathcal{R}\}$ *is* weakly reversible *if for any reaction* $(\nu \to \nu') \in \mathcal{R}$ *there exists a sequence of reactions from* $\mathcal{R}$ *starting with* ν' *as a source complex and ending with* ν *as a product complex, i.e. there exist complexes* $\nu_1, ..., \nu_m \in \mathcal{C}$ *such that*

$$\left(\nu' \to \nu_1\right), (\nu_1 \to \nu_2), \ldots, (\nu_{m-1} \to \nu_m), (\nu_m \to \nu) \in \mathcal{R}.$$

A CRN $\{\mathcal{S}, \mathcal{C}, \mathcal{R}\}$ *is* reversible *if* $(\nu \to \nu') \in \mathcal{R}$ *implies* $(\nu' \to \nu) \in \mathcal{R}$.

To each CRN we associate in a one-to-one fashion a directed graph $\mathcal{G} = \mathcal{G}(\mathcal{S}, \mathcal{C}, \mathcal{R})$ as follows: the nodes of the graph are the complexes $\mathcal{C}$. Two complexes $\nu, \nu' \in \mathcal{C}$ are connected by a directed edge if and only if $(\nu \to \nu') \in \mathcal{R}$.

Each connected component of $\mathcal{G}$ is called a *linkage class* of $\mathcal{G}$. We denote the number of linkage classes in $\mathcal{G}$ by $\ell(\mathcal{G})$. A CRN is weakly reversible if and only if each linkage class of $\mathcal{G}$ is weakly reversible.

Definition 2 (stoichiometric subspace and compatibility classes)**.** *The space*

$$\Sigma = \operatorname{span}\{\eta_s\}_{s=1}^R \subset \mathbb{Z}^d$$

is called the stoichiometric subspace *of the CRN* $(\mathcal{S}, \mathcal{C}, \mathcal{R})$*. Its dimension* $\dim \Sigma$ *is called the* rank *of the CRN* $(\mathcal{S}, \mathcal{C}, \mathcal{R})$*.*

For a vector $c \in \mathbb{R}^d$*, the affine subspace* $c + \Sigma$ *and the set* $(c + \Sigma) \cap \mathbb{R}^d_{>0}$ *are referred to as* stoichiometric compatibility class *and* positive stoichiometric compatibility classes *of the CRN, respectively.*

Definition 3 ([15])**.** *The* deficiency δ *of a CRN* $\{\mathcal{S}, \mathcal{C}, \mathcal{R}\}$ *with a graph* $\mathcal{G} = \mathcal{G}(\mathcal{S}, \mathcal{C}, \mathcal{R})$ *is*

$$\delta = \#\mathcal{C} - \ell(\mathcal{G}) - \dim \Sigma.$$

For any CRN it holds that $\delta \in \mathbb{Z}_{\geq 0}$, see [18, (2.11)].

Although the aforesaid relates to chemical systems and, correspondingly, to chemical reaction networks, the discussion and results are applicable to general systems driven by Markov processes. We refer to [24] for examples in modelling migration, queuing networks and clustering

processes. The general assumption made on the corresponding systems is the *spatial homogeneity*, which requires, irrespective of the dynamics, that the reactions are equally likely to occur at every spatial point and their kinetics allows for the system to relax between reactions and remain spatially homogeneous. This assumption justifies the use of the spatially homogeneous stochastic model that we describe in Section 2.3. For chemical and biochemical systems, it means that the systems are *well stirred* and their dynamics follow paths of *thermal equilibrium*. For an overview of the models used in systems biology we refer to [25].

2.2 Dynamical models

In the mathematical modelling of biochemical processes in living organisms, two broad classes of mathematical models for CRNs are distinguished: deterministic and stochastic. In the small volume and low copy number regime which is of particular interest in systems biology, stochastic mathematical models are widely used in descriptions of the dynamics of CRNs. These models account for fluctuations in chemical reactions and in copy number counts which are induced, for example, by thermal noise. In the large volume and large copy number regime asymptotic analysis (see, for example, [26]) justifies the use of deterministic models to account for the time evolution of mean concentrations of the species.

While being at the opposite extremes of scales, both types of models in certain cases share fundamental mathematical features (depending solely on the algebraic structure of the CRN) which entail, as we shall show in this paper, that tensor-structured approximations of the probability density function describing the system under stochastic models converge with *linear scaling* with respect to the number d of species and with logarithmic scaling with respect to the approximation accuracy ε as well as with logarithmic scaling in terms of the maximum copy numbers considered in a finitely truncated state space.

2.3 Stochastic model

The dynamics of a system with a CRN $\{\mathcal{S}, \mathcal{C}, \mathcal{R}\}$ introduced above can be modelled as continuous time Markov chain X with state space $\mathcal{Z} = \mathbb{Z}^d_{\geq 0}$, which describes the system's state at time t in terms of a vector $X(t)$ composed of the copy numbers of the species at time t. Accordingly, $X(t)$ is modelled as a cadlag stochastic process with discontinuous dependence on time: if the sth reaction occurs at time t, then

$$X(t) = \lim_{\tau \downarrow 0} X(t - \tau) + \eta_s \,.$$

Denoting with $S_s(t)$ the stochastic process counting the occurrences of the sth reaction up to time t, we write

$$X(t) = X(0) + \sum_{s=1}^{R} S_s(t)\, \eta_s \,, \tag{1}$$

where $S_s(t)$ is a *Cox counting process* with rate $\omega_s(X(t))$. For $1 \leq s \leq R$, the function ω_s comes from the model of the sth reaction and, in the case of a chemical system, is called the *propensity (function)* of the reaction. For $1 \leq s \leq R$ the process $S_s(t)$ can be represented as

$$S_s(t) = Z_s\left(\int_0^t \omega_s(X(\tau))\, \mathrm{d}\tau \right) \,, \tag{2}$$

$\{Z_s\}_{s=1}^R$ being independent rate-one Poisson processes. Let us for all $t \geq 0$ define the *transition operator* $\boldsymbol{P}(t) : [0,1]^{\mathcal{Z}} \to [0,1]^{\mathcal{Z}}$ by setting

$$\boldsymbol{P}_{ij}(t) = \mathbb{P}\left\{ X(t) = j \mid X(0) = i \right\} \quad \text{for} \quad i, j \in \mathcal{Z}.$$

The family of transition operators $\{\boldsymbol{P}(t)\}_{t \geq 0}$ is a commutative semi-group with *infinitesimal generator* $\boldsymbol{Q}$ given by an infinite matrix with entries

$$\boldsymbol{Q}_{ij} = \lim_{t \downarrow 0} \frac{\boldsymbol{P}_{ij}(t) - \delta_{ij}}{t}, \quad \text{where} \quad i, j \in \mathcal{Z}.$$

Then the *probability density function (PDF)* $\boldsymbol{p} : [0,\infty) \to [0,1]^{\mathcal{Z}}$ of the process X, given by $\boldsymbol{p}_j(t) = \mathbb{P}\{X(t) = j\}$ for $j \in \mathcal{Z}$ and $t \geq 0$, satisfies the *Chapman–Kolmogorov* (alternatively, *forward Kolmogorov*) equation

$$\dot{\boldsymbol{p}}(t) = \boldsymbol{A}\,\boldsymbol{p}(t)\,, \quad t \geq 0, \tag{3}$$

referred to as the *chemical master equation (CME)* in the context of chemical systems, where $\boldsymbol{A} = \boldsymbol{Q}^{\top}$ is called the *CME operator*. For the dynamics given by (1)–(2), the calculation of the infinitesimal generator yields for all $\boldsymbol{q} \in [0,1]^{\mathcal{Z}}$

$$(\boldsymbol{Q}\,\boldsymbol{q})_{\,i} = \sum_{s=1}^{R} \boldsymbol{\omega}_{s\,i} \cdot (\boldsymbol{q}_{i+\eta_s} - \boldsymbol{q}_i)\,, \quad i \in \mathcal{Z}, \tag{4}$$

where for $1 \leq s \leq R$ with $\boldsymbol{\omega}_s \in \mathbb{R}^{\mathcal{Z}}_{\geq 0}$ we denote the sth *propensity vector* given by

$$\boldsymbol{\omega}_{s\,i} = \omega_s(i)\,, \quad i \in \mathcal{Z}. \tag{5}$$

Therefore

$$\boldsymbol{Q} = \sum_{s=1}^{R} (\operatorname{diag}\boldsymbol{\omega}_s) \cdot (\boldsymbol{S}_{-\eta_s} - \mathbb{I})\,, \quad \boldsymbol{A} = \sum_{s=1}^{R} (\boldsymbol{S}_{\eta_s} - \mathbb{I}) \cdot \operatorname{diag}\boldsymbol{\omega}_s, \tag{6}$$

where $\boldsymbol{S}_{\eta_s}$ is the matrix of downward η_{sk}-position shift in the kth dimension, $1 \leq k \leq d$, for $1 \leq s \leq R$.

Every initial state $X(0) = c \in \mathcal{Z}$ of the Markov process X corresponds to a positive stoichiometric compatibility class of reachable states in the sense of Definition 2. Also, we are particularly interested in those subsets of such classes, which are *closed, irreducible communicating (equivalence) classes* of X.

As we see from (3), every stationary distribution

$$\boldsymbol{p}(\infty) = \lim_{t\to\infty} \boldsymbol{p}(t)$$

of the process X belongs to the kernel of the CME operator (6). When the CRN is weakly reversible and has zero deficiency in the sense of Feinberg, the process X, within each irreducible communicating equivalence class, has a unique product-form stationary distribution given by Theorem 5. Numerically this unique distribution can be obtained approximately by computing the kernel of the CME operator or by modelling the evolution of the PDF till large times. These methods have to be applied to a properly truncated system with a finite state space $\mathcal{Z}_n \subset \mathcal{Z}$, see Section 2.6 below. However, for truncations of reasonable accuracy the finite subset $\mathcal{Z}_n$ may be unaffordably large. In this respect, the major challenge is the *curse of dimensionality*, which shows up as the exponential growth with respect to d of the cardinality of $\mathcal{Z}_n$ and, consequently, of the number of entries in the truncated PDF $\hat{\boldsymbol{p}}$ and CME operator $\hat{\boldsymbol{A}}$. In [14, 13] this challenge was taken up with the use of the *tensor train (TT)* and *quantized tensor train (QTT)* decompositions of multidimensional arrays (such as $\hat{\boldsymbol{p}}$ and $\hat{\boldsymbol{A}}$), or *tensors*. Those decompositions, introduced briefly in Section 3.1 below, are adaptive nonlinear low-parametric approximations of tensors, based on the separation of variables and providing a format with robust and efficient arithmetics.

This paper focuses on the QTT structure of the truncated stationary PDF and of the truncated CME operator. Theorem 5, which was proved in [16], implies that the unique stationary distribution is of the product form, which means that the analysis of the QTT structure of the distribution reduces to that of the univariate factors of the distribution.

2.4 Admissible propensity functions

To complete the model presented in Section 2.3, we have to specify the models of the reactions, i.e. the propensity functions $\{\omega_s : \mathcal{Z} \to \mathbb{R}_{\geq 0}\}_{s=1}^{R}$. We assume that each is of the form

$$\omega_s(i) = \kappa_s \,\frac{\theta(i)}{\theta(i-\nu_k)} \prod_{k=1}^{d} \mathbf{1}_{\mathcal{X}_{sk}}(i_k)\,, \quad i \in \mathcal{Z}, \tag{7}$$

where $\kappa_s > 0$ is the *rate* of the sth reaction and $\mathcal{X}_{sk} = \mathbb{Z}_{\geq \nu_{sk}}$ for $1 \leq k \leq d$, so that $\times_{k=1}^{d} \mathcal{X}_{sk} \subset \mathcal{Z}$ is the set of states in which there are enough copies of all species in the system for the sth reaction to occur. Further, we assume that

$$\theta(i) = \prod_{k=1}^{d} \prod_{j_k=1}^{i_k} \theta_k(j_k)\,, \quad i \in \mathcal{Z}, \tag{8}$$

where the function θ_k represents the interaction rate of the kth species and can be interpreted as its "rate of association" in a broad sense. Then the propensity (7) takes the separable form

$$\omega_s(i) = \kappa_s \prod_{k=1}^{d} \mathbf{1}_{\mathcal{X}_{sk}}(i_k) \cdot \omega_{sk}(i_k)\,, \quad i \in \mathcal{Z}, \tag{9}$$

where, for $1 \leq s \leq R$ and $1 \leq k \leq d$, the propensity factor ω_{sk} reads as

$$\omega_{sk}(i_k) = \prod_{j_k=0}^{\nu_{sk}-1} \theta_k(i_k - j_k)\,, \quad i_k \in \mathbb{Z}_{\geq 0}. \tag{10}$$

In the present paper we consider two types of kinetics given by particular functions $\{\theta_k\}_{k=1}^{d}$. First, under the *stochastic mass action kinetics* for the kth species we consider

$$\theta_k(i_k) = i_k, \quad i_k \in \mathbb{Z}_{\geq 0}, \tag{11}$$

which leads to the propensity factors

$$\omega_{sk}(i_k) = \nu_{sk}! \binom{i_k}{\nu_{sk}} = \frac{i_k!}{(i_k - \nu_{sk})!}, \quad i_k \in \mathbb{Z}_{\geq 0}. \tag{12}$$

Alternatively, under the *stochastic Michaelis–Menten kinetics* for the kth species we assume

$$\theta_k(i_k) = \frac{\vartheta_k i_k}{\upsilon_k + i_k}, \quad i_k \in \mathbb{Z}_{\geq 0}, \tag{13}$$

with a constant $\vartheta_k > 0$ and an integer constant $\upsilon_k \geq 0$, which results in

$$\omega_{sk}(i_k) = \vartheta_k^{\nu_{sk}} \prod_{j_k=0}^{\nu_{sk}-1} \frac{i_k - j_k}{\upsilon_k + i_k - j_k}, \quad i_k \in \mathbb{Z}_{\geq 0}. \tag{14}$$

The mass action kinetics law is assumed in many models, including those for chemical systems; see [24]. The Michaelis–Menten law is a simple model for enzymatic reactions where the reaction rate is limited by the amount of enzyme present and saturates to ϑ_k, see [27, Chapter 1] and [24, Chapter 8.5] for details. Arbitrary combinations of the above choices (11), (13) for the factors $\{\theta_k\}_{k=1}^{d}$ may appear in mixed propensity models of the form (7)–(8). In either case, the propensity vectors (5) take the Kronecker-product form

$$\boldsymbol{\omega}_s = \boldsymbol{\omega}_{s1} \otimes \ldots \otimes \boldsymbol{\omega}_{sd}\,, \quad 1 \leq s \leq R\,, \tag{15}$$

where the univariate factors are vectors composed of the values of (10).

2.5 Deterministic Model

As outlined in Section 2.3, the solution of the CME describes the evolution of the system under a stochastic model. However, when all species are present in large copy numbers, the effect of stochasticity is less significant and the evolution of the system can be described by the solution of a deterministic nonlinear ODE on the state space $\mathbb{R}^d_{\geq 0}$. This approximation is based on the scaling with respect to a system size parameter and boils down to modelling the evolution

of concentrations $x = (x_1, \ldots, x_d)^\top \in \mathbb{R}^d_{\geq 0}$ of the species instead of that of the PDF with respect to all possible copy numbers $X = (X_1, \ldots, X_d)^\top \in \mathbb{Z}^d_{\geq 0}$. We refer to [26, 28, 29] for details. Under such an approximation, the stochastic model with the mass-action, Michaelis–Menten or mixed kinetics transforms to the corresponding deterministic system given by

$$x(t) = x(0) + \sum_{s=1}^{R} \eta_s \int_0^t f_s(x(\tau))\,\mathrm{d}\tau, \quad \text{or} \quad \dot{x}(t) = \sum_{s=1}^{R} \eta_s f_s(x(t))\,, \tag{16}$$

for all $t > 0$. The rate functions are given for $1 \leq s \leq R$ by

$$f_s(x) = \kappa_s \prod_{k=1}^{d} x_k^{\nu_{sk}}, \quad x \in \mathbb{R}^d_{\geq 0}\,. \tag{17}$$

Definition 4. *A vector $c \in \mathbb{R}^d_{\geq 0}$ satisfying*

$$\sum_{\substack{1 \leq s \leq R: \\ \nu_s = \xi}} f_s(c) = \sum_{\substack{1 \leq s \leq R: \\ \nu'_s = \xi}} f_s(c) \quad \textit{for all} \quad \xi \in \mathcal{C}, \tag{18}$$

is called a complex-balanced equilibrium *of the deterministic system* (16)–(17).

The condition (18) means that in every complex-balanced equilibrium state c the complex formation is zero for all complexes. In particular, the right-hand side of (16) becomes zero, therefore c is a steady state of (16)–(17). Complex-balanced equilibria are admitted for arbitrary positive rate constants $\{\kappa_s\}_{s=1}^R$ by a system of zero deficiency only if the corresponding CRN is weakly reversible, see [15, Remark 5.2]. When it is, such a system allows, within every positive stoichiometric compatibility class, precisely one steady state [15, Corollary 5.4]. This steady state is a complex-balanced equilibrium of the system, asymptotically stable with respect to its stoichiometric compatibility class [15, Remark 5.4]. These statements constitute a substantial part of Feinberg's deficiency zero theorem, see [15, Theorem 5.1] or [18, Theorem 6.1.1] and are the foundation of the analysis of the relation between the stochastic and deterministic models. The existence of a complex-balanced equilibrium is assumed in [16, Theorem 6.1] stated below. This result is the starting point of the analysis in the present paper.

Theorem 5 (Theorem 6.1 in [16])**.** *Suppose that the deterministic model* (16)–(17)*, corresponding to the stochastic model given by* (1)–(2) *and* (7)–(8)*, admits a complex-balanced equilibrium $c \in \mathbb{R}^d_{>0}$. Then*

(a) the stochastic model admits the stationary distribution $\boldsymbol{p}$ given by

$$\boldsymbol{p}_i = M \prod_{k=1}^{d} \frac{c_k^{i_k}}{\prod_{j_k=1}^{i_k} \theta_k(j_k)}, \tag{19}$$

where $M > 0$ is a normalization constant, for $i \in \mathcal{Z}$, provided that $\boldsymbol{p}$ is summable; if $\mathcal{Z}$ is an irreducible communicating class of X, then $\boldsymbol{p}$ is a unique stationary distribution;

(b) for every closed, irreducible communicating class $\mathfrak{G} \subset \mathcal{Z}$ of X the stochastic model admits the stationary distribution $\boldsymbol{p}$ given by (19) *for $i \in \mathfrak{G}$ with an appropriate normalization constant $M > 0$ and zero outside $\mathfrak{G}$, provided that $\boldsymbol{p}$ is summable.*

For the mixed mass-action and Michaelis–Menten kinetics given by (11) and (13) respectively, Theorem 5 suggests a stationary distribution of the form

$$\boldsymbol{p} = M \cdot \boldsymbol{p}_1 \otimes \ldots \otimes \boldsymbol{p}_d, \tag{20}$$

where each factor is given for all $i_k \in \mathbb{Z}_{\geq 0}$ by either

$$\boldsymbol{p}_{k\,i_k} = \frac{c_k^{i_k}}{i_k!} \quad \text{or} \quad \boldsymbol{p}_{k\,i_k} = \left(\frac{c_k}{\vartheta_k}\right)^{i_k} \frac{(\upsilon_k + i_k)!}{\upsilon_k!\, i_k!}, \tag{21}$$

depending on the kinetics of the kth species.

2.6 Finite state projection

The CME (3) is posed on the (countably) infinite set of states $\mathcal{Z} = \mathbb{Z}^d_{\geq 0}$. In order to be able to address general systems computationally, Munsky and Khammash proposed the Finite State Projection Algorithm (FSP) [10, 11] which seeks to truncate the countably infinite dimensional space $\mathcal{Z}$ of states of the process to a finite subset over which the dynamics are close to those of the original system.

With a multi-index $n = (n_1, n_2, ..., n_d) \in \mathbb{N}^d$ we associate the finite set $\mathcal{Z}_n$ of states, defined as follows:

$$\mathcal{Z}_n = \{i \in \mathcal{Z} : 0 \leq i_k < n_k \quad \text{for} \quad 1 \leq k \leq d\} \subset \mathcal{Z} \,. \tag{22}$$

Theorem 6 (FSP, Theorem 2.2 in [11])**.** *Consider a Markov process with state space $\mathcal{Z} = \mathbb{Z}^d_{\geq 0}$, the PDF of which evolves on $[0, \infty)$ according to (3) and satisfies the initial condition $\boldsymbol{p}(0) = \boldsymbol{p}_0$ for some $\boldsymbol{p}_0 \in [0,1]^{\mathcal{Z}}$ supported in $\mathcal{Z}_n$. Let $\hat{\boldsymbol{A}} \in \mathbb{R}^{\mathcal{Z}_n \times \mathcal{Z}_n}$ denote the restriction of $\boldsymbol{A}$ to $\mathcal{Z}_n$. Denote by $t \mapsto \hat{\boldsymbol{p}}(t) \in [0,1]^{\mathcal{Z}_n}$ the solution of the FSP truncated system with dynamics given by the linear autonomous ODE*

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\boldsymbol{p}}(t) = \hat{\boldsymbol{A}}\hat{\boldsymbol{p}}(t)\,, \quad t \geq 0, \tag{23}$$

satisfying the initial condition $\hat{\boldsymbol{p}}(0) = \boldsymbol{p}_0|_{\mathcal{Z}_n}$. Then, if for some $\epsilon > 0$ and $t \geq 0$

$$\sum_{i \in \mathcal{Z}_n} \hat{\boldsymbol{p}}_j(t) \geq 1 - \epsilon, \tag{24}$$

then $\hat{\boldsymbol{p}}_i(t) \leq \boldsymbol{p}_i(t) \leq \hat{\boldsymbol{p}}_i(t) + \epsilon$ for every $i \in \mathcal{Z}_n$ and

$$\left\| \hat{\boldsymbol{p}}(t) - \boldsymbol{p}(t)\,|_{\mathcal{Z}_n} \right\|_1 \leq \epsilon. \tag{25}$$

Assuming that a FSP has been performed, we henceforth treat $\boldsymbol{p}$ as a d-dimensional $n_1 \times \ldots \times n_d$-vector, i.e. as an array, or *tensor*, indexed by $i = (i_1, \ldots, i_d) \in \mathcal{Z}_n$. Each dimension k (alternatively referred to as a *mode* or *level*) has a corresponding *mode size* n_k, which is the number of values which the index for that dimension can take. Clearly, $n_k - 1$ is the maximum copy number of the kth species, considered within the FSP.

For a truncation satisfying (24), the estimate (25) gives an explicit certificate of the accuracy of the approximate solution. In practice, the truncation required to satisfy a given error tolerance may still require a very large number of states: the number of entries in the truncated PDF $\hat{\boldsymbol{p}}$ equals $\#\mathcal{Z}_n = \prod_{k=1}^d n_k$, which renders the direct numerical simulation of even the projected CME (23) or of the corresponding steady-state problem infeasible in many cases. In [14] a novel approach for the numerical solution of such FSP truncated systems that retain large numbers of states was proposed, one of the key ideas being the use of the QTT format for representing $\hat{\boldsymbol{p}}$ and $\hat{\boldsymbol{A}}$ in terms of much fewer than $\#\mathcal{Z}_n$ parameters.

For notational convenience, we drop the superscripts n and the hat from $\hat{\boldsymbol{p}}$ indicating the FSP since we will only consider systems which have already been truncated. Similarly, we deal with restricted propensity vectors (5), their univariate components in (15), and shift operators in (6) without change of notation.

The remainder of the present paper is a brief outline of the TT and QTT formats and the rank-accuracy analysis of the QTT structure, first, of the truncated CME operator (6) for the mass-action, Michaelis–Menten or mixed kinetics (which extends the results of [14]) and, second, of the truncated stationary distribution (20) of the corresponding system, which it has under the assumptions of Theorem 5.

3 TT and QTT decompositions

3.1 Tensor train representation

By *tensors* we mean multidimensional arrays, vectors and matrices being notable examples. To compute stationary solutions of the CME (3) under accurate FSP truncations and for large

d efficiently, we propose to use the *tensor train* (TT for short) decomposition, a non-linear low-parametric representation of multidimensional arrays based on the separation of variables, developed by Oseledets and Tyrtyshnikov [30, 31].

First, let us consider a d-dimensional $n_1 \times \ldots \times n_d$-vector $\boldsymbol{p}$. If two- and three-dimensional arrays $U_1, U_2, \ldots, U_d$ satisfy the equation

$$\boldsymbol{p}_{j_1,\ldots,j_d} = \sum_{\alpha_1=1}^{r_1} \cdots \sum_{\alpha_{d-1}=1}^{r_{d-1}} U_1(j_1, \alpha_1) \cdot U_2(\alpha_1, j_2, \alpha_2) \cdot \ldots \cdot U_{d-1}(\alpha_{d-2}, j_{d-1}, \alpha_{d-1}) \cdot U_d(\alpha_{d-1}, j_d) \tag{26}$$

for $0 \le j_k \le n_k - 1$, where $1 \le k \le d$, then $\boldsymbol{p}$ is said to be represented in the TT decomposition in terms of the *core tensors* $U_1, U_2, \ldots, U_d$. The summation indices $\alpha_1, \ldots, \alpha_{d-1}$ and limits $r_1, \ldots, r_{d-1}$ on the right-hand side of (26) are called, respectively, *rank indices* and *ranks* of the representation. A TT decomposition, exact or approximate, can be constructed via the low-rank representation of a sequence of single matrices; for example, with the help of the SVD. In particular, for every $k = 1, \ldots, d-1$ the representation (26) implies a rank-r_k factorization of an *unfolding matrix* $\boldsymbol{U}^{(k)}$ with the entries

$$\boldsymbol{U}^{(k)}_{\overline{j_1,\ldots,j_k};\,\overline{j_{k+1},\ldots,j_d}} = \boldsymbol{p}_{j_1,\ldots,j_k,j_{k+1},\ldots,j_d}.$$

Conversely, if the vector $\boldsymbol{p}$ is such that the unfolding matrices $\boldsymbol{U}^{(1)}, \ldots, \boldsymbol{U}^{(d-1)}$ are of ranks $r_1, \ldots, r_{d-1}$ respectively, then the cores $U_1, U_2, \ldots, U_d$ satisfying (26) do exist; see Theorem 2.1 in [31]. The ranks of the unfolding matrices are the lowest possible ranks of a TT decomposition of the vector. They are hence referred to as *TT ranks of the vector*.

Another, fundamental, property of the TT representation is that if the unfolding matrices can be approximated with ranks $r_1, \ldots, r_{d-1}$ and accuracies $\varepsilon_1, \ldots, \varepsilon_{d-1}$ in the Frobenius norm, then the vector itself can be approximated in the TT format with ranks $r_1, \ldots, r_{d-1}$ and accuracy $\sqrt{\sum_{k=1}^{d-1} \varepsilon_k^2}$ in the ℓ_2-norm. This underlies a robust and efficient algorithm for the low-rank TT approximation of vectors given in full format or in the TT format with higher ranks. For details see Theorem 2.2 with corollaries and Algorithms 1 and 2 in [31]. In practice it may be essential that the TT representation relies on a certain ordering of the dimensions and *reordering dimensions may affect the numerical values of the TT ranks significantly*.

The multiplication of a vector given in the TT decomposition (26) by a d-dimensional $(m_1 \times \ldots \times m_d) \times (n_1 \times \ldots \times n_d)$-matrix $\boldsymbol{A}$ can be performed efficiently if the matrix is represented as follows:

$$\boldsymbol{A}_{i_1,\ldots,i_d j_1,\ldots,j_d} = \boldsymbol{a}_{\overline{i_1,j_1},\ldots,\overline{i_d,j_d}} = \sum_{\alpha_1=1}^{r_1} \cdots \sum_{\alpha_{d-1}=1}^{r_{d-1}} V_1(i_1, j_1, \alpha_1) \cdot V_2(\alpha_1, i_2, j_2, \alpha_2) \cdot \ldots \cdot V_{d-1}(\alpha_{d-2}, i_{d-1}, j_{d-1}, \alpha_{d-1}) \cdot V_d(\alpha_{d-1}, i_d, j_d)\,, . \tag{27}$$

The decomposition (27) is called a TT representation of the matrix $\boldsymbol{A}$, the TT cores $V_1, \ldots, V_d$ are now three- and four-dimensional arrays. The discussion of the efficiency and robustness of the TT decomposition of vectors also applies to the matrix case. Indeed, (27) can be interpreted as a TT decomposition of a vectorization of $\boldsymbol{A}$, in which the corresponding row and column indices are merged to obtain a d-dimensional $m_1 \cdot n_1 \times \ldots \times m_d \cdot n_d$-vector.

Basic operations of linear algebra with vectors and matrices in the TT format, such as addition, Hadamard and dot products, multi-dimensional contraction, matrix-vector multiplication, etc. are considered in detail in [31]. The use of tensor-structured approximations aims primarily at reducing the complexity of computations and avoiding the curse of dimensionality. The TT format potentially achieves this with the storage cost and complexity of basic operations of the TT arithmetics, applied to the representation of the form (26), being bounded by dnr^α with $\alpha \in \{2, 3\}$, where $n \ge n_1, \ldots, n_d$ and $r \ge r_1, \ldots, r_{d-1}$. This estimate is formally linear in d; however, the TT ranks $r_1, \ldots, r_{d-1}$ in (26) may depend on d and n.

So far there has been increasing, mostly experimental, evidence that in many applications the TT and QTT ranks are moderate, e.g. are either constant or grow linearly with respect to d and are either constant or grow logarithmically with respect to n, which is crucial for the applicability of TT- and QTT-structured methods. For examples see the papers [32, 33, 34, 35, 36, 13, 14] and the extensive survey [37].

3.2 Quantized tensor train representation

With the aim of further reduction of the complexity, the TT format can be applied to a *quantized* tensor, which leads to the *Quantized Tensor Train (QTT)* format [21, 23, 22]. The idea of *quantization* consists in "folding" the vector (matrix) by introducing l_k "virtual" dimensions (levels) corresponding to the k-th "physical" dimension [38], provided that the corresponding mode size n_k can be factorized as $n_k = n_{k,1} \cdot n_{k,2} \cdot \ldots \cdot n_{k,l_k}$ in terms of integral factors $n_{k,1}, \ldots, n_{k,l_k} \geq 2$, for $1 \leq k \leq d$. This transformation can be viewed as reshaping the k-th mode of size n_k into l_k modes of sizes $n_{k1}, \ldots, n_{k,l_k}$.

Under quantization applied to all dimensions, a d-dimensional $n_1 \times \ldots \times n_d$-vector indexed by $j_1 = \overline{j_{1,1}, \ldots, j_{1,l_1}}, \ldots, j_d = \overline{j_{d,1}, \ldots, j_{d,l_d}}$ is transformed into an $l_1 + \ldots + l_d$-dimensional $n_{1,1} \times \ldots \times n_{1,l_1} \times \ldots\ldots \times n_{d,1} \times \ldots \times n_{d,l_d}$-vector indexed by $j_{1,1}, \ldots, j_{1,l_1}, \ldots\ldots, j_{d,1}, \ldots, j_{d,l_d}$. With the overscore we denote vectorized multi-indices: $\overline{j_{k,1}, \ldots, j_{k,l_k}} = \sum_{m=1}^{l_k} i_{k,m} \prod_{\ell=k+1}^{l_k} n_{k,\ell}$ for $1 \leq k \leq d$. By a *QTT decomposition* of a vector and the *QTT ranks of the decomposition* we mean a TT decomposition of its quantization and the ranks of that TT decomposition.

Example 7 (Proposition 1.1 in [23])**.** *To demonstrate how the quantization reduces complexity of structured data, let us consider the one-dimensional vector* $\boldsymbol{p} = \left(1, q, \ldots, q^{2^l-1}\right)^\top$ *. This vector has a single "physical" dimension, and its elementwise representation requires storing* 2^l *parameters. However, if we apply the quantization transformation as described above to split the single dimension into* l *virtual levels,* $\boldsymbol{p}$ *is transformed into an* l*-dimensional vector that exhibits a low-parametric structure. Indeed, in terms of the "virtual" indices it is a rank-one Kronecker product of* l *vectors with* 2 *components each:*

$$\boldsymbol{p} = \begin{pmatrix} 1 \\ q^{2^{l-1}} \end{pmatrix} \otimes \begin{pmatrix} 1 \\ q^{2^{l-2}} \end{pmatrix} \otimes \ldots \otimes \begin{pmatrix} 1 \\ q \end{pmatrix},$$

which implies a QTT decomposition of $\boldsymbol{p}$ *with ranks* $1, \ldots, 1$*. Other explicit low-rank examples can be found in [39, 40, 41, 42].*

When the natural ordering

$$\underbrace{j_{1,1}, \ldots, j_{1,l_1}}_{\text{1st dimension}}, \underbrace{j_{2,1}, \ldots, j_{2,l_2}}_{\text{2nd dimension}}, \ldots\ldots, \underbrace{j_{d,1}, \ldots, j_{d,l_d}}_{d\text{th dimension}} \tag{28}$$

of the "virtual" indices is used for representing the quantized vector in the TT format, the ranks of the QTT decomposition can be enumerated as follows:

$$\underbrace{r_{1,1}, \ldots, r_{1,l_1-1}}_{\text{1st dimension}}, \hat{r}_1, \underbrace{r_{2,1}, \ldots, r_{2,l_2-1}}_{\text{2nd dimension}}, \hat{r}_2, \ldots\ldots, \hat{r}_{d-1}, \underbrace{r_{d,1}, \ldots, r_{d,l_d-1}}_{d\text{th dimension}},$$

where $\hat{r}_1, \ldots, \hat{r}_{d-1}$ are the TT ranks of the original tensor, i.e. the ranks of the separation of "physical" dimensions. That is, the TT ranks of a tensor are some of the QTT ranks of the same tensor.

In this sense (26) and (27), with d being replaced with l, also present QTT representations of ranks $r_1, \ldots, r_{l-1}$ of a one-dimensional vector $\tilde{\boldsymbol{p}}$ and of a one-dimensional matrix $\tilde{\boldsymbol{A}}$ with entries $\tilde{\boldsymbol{p}}_{\overline{j_1,\ldots,j_l}} = \boldsymbol{p}_{j_1,\ldots,j_l}$ and $\tilde{\boldsymbol{A}}_{\overline{i_1,\ldots,i_l j_1,\ldots,j_l}} = \boldsymbol{A}_{i_1,\ldots,i_l j_1,\ldots,j_l}$ respectively. Since a QTT decomposition is a TT representation of an appropriately quantized tensor, the structure of basic operation in the TT format and related algorithms, referred to in Section 3.1, when applied to QTT decompositions,

naturally provide the same in the QTT format. Compared to the TT representation, the QTT format is seeks to resolve more structure in the data by splitting additionally the "virtual" dimensions introduced by quantization. To exploit this as much as possible, we use and consider in the rest of the paper as fine a quantization (i.e. with small n_{k,m_k}) as possible. This choice maximizes the number of virtual modes. From now on, for each mode size n_k we assume that $n_k = 2^{l_k}$ for $1 \le k \le d$ and consider the *ultimate binary quantization* with $n_{k,m_k} = 2$ for all m_k and k, so that $j_k = \overline{j_{k,1}, \ldots, j_{k,l_k}} = \sum_{m_k=1}^{l_k} 2^{l_k - m_k} j_{k,m_k}$, where the indices $j_1, \ldots, j_l$ take the values 0 and 1.

The storage cost and complexity of basic QTT-structured operations are bounded from above by

$$d\, l\, r^{\alpha} \tag{29}$$

with $\alpha \in \{2, 3\}$, where $l \ge l_1, \ldots, l_d$ and r is an upper bound on all QTT ranks of the decomposition in question. Note that this estimate may be, depending on r, logarithmic in $n = 2^l$ and also in $n^d = 2^{dl}$, which is an upper bound on the number of entries.

Note that the *Hierarchical Tensor Representation* [43, 44] itself and combined with *tensorization* [45], a comprehensive exposition of which is given in [46], are closely related counterparts of the TT and QTT formats respectively. Also, the TT representation, in fact, is known as *Matrix Product States (MPS)* and has been exploited by physicists to describe quantum spin systems theoretically and numerically for at least two decades now, see [47, 48, 49].

3.3 Preliminaries for the QTT-structured approximation

Proposition 8 (Sections 4.1 and 4.2 in [31]). *Assume that $\boldsymbol{p}$ and $\boldsymbol{q}$ are d-dimensional tensors of equal mode sizes, given in TT representations of ranks $p_1, \ldots, p_d$ and $q_1, \ldots, q_d$ respectively. Then for all $\alpha, \beta \in \mathbb{R}$ the linear combination $\alpha\boldsymbol{p} + \beta\boldsymbol{q}$ has a TT decomposition of ranks $p_1 + q_1, \ldots, p_d + q_d$. On the other hand, the Hadamard product $\boldsymbol{p} \odot \boldsymbol{q}$ can be represented in the TT format with ranks $p_1 q_1, \ldots, p_{d-1} q_{d-1}$.*

Proposition 9. *If a vector $\boldsymbol{p}$ is given in the TT format with certain ranks, then its diagonalization* $\operatorname{diag} \boldsymbol{p}$ *can be represented in the TT format with the same ranks.*

Proof. It is enough to note that under the diagonalization of a vector each TT core is diagonalized with respect to the corresponding mode index. □

Proposition 10 (Section 4.3 in [31]). *If matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ have TT representations of ranks $p_1, \ldots, p_{d-1}$ and $q_1, \ldots, q_{d-1}$ respectively, their product $\boldsymbol{AB}$, when it is defined, has a TT representation of ranks $p_1 q_1, \ldots, p_{d-1} q_{d-1}$.*

Proposition 11 (Section 3.1 in [31]). *Consider vectors $\boldsymbol{p}$ and $\boldsymbol{q}$ given in TT decompositions of ranks $p_1, \ldots, p_{d-1}$ and $q_1, \ldots, q_{l-1}$ respectively. The tensor product $\boldsymbol{p} \otimes \boldsymbol{q}$ can be represented in the TT format with ranks $p_1, \ldots, p_{d-1}$, 1, $q_1, \ldots, q_{l-1}$.*

Lemma 12. *Let $l, J \in \mathbb{N}$, $\nu = \{\nu_j\}_{j=0}^{J} \subset \mathbb{Z} :\ 0 = \nu_0 < \nu_1 < \ldots < \nu_J = 2^l$ and $a = \{a_j\}_{j=1}^{J} \subset \mathbb{C}$. Then the 2^l-component vector $\boldsymbol{\sigma}$ given by*

$$\boldsymbol{\sigma}_i = a_j, \quad \nu_{j-1} \le i < \nu_j,$$

for $1 \le j \le J$ has a QTT representation of ranks bounded by J.

Proof. For $1 \le k \le l-1$ let $\boldsymbol{U}^{(k)}$ be the kth unfolding matrix of $\boldsymbol{\sigma}$:

$$\boldsymbol{U}^{(k)}{}_{\overline{i_l, \ldots, i_{k+1} i_k, \ldots, i_1}} = \boldsymbol{\sigma}_{\overline{i_l, \ldots, i_1}} \quad \text{for} \quad i_m \in \{0, 1\},\ 1 \le m \le l.$$

This matrix may have at most $J - 1$ rows consisting of at least two different values of a. Every other row is filled with only one element of $\{a_j\}_{j=1}^{J}$. Therefore there are at most J linearly independent rows in the matrix. Thus, $\operatorname{rank} \boldsymbol{U}^{(k)} \le J$. This bound, which is valid for $1 \le k \le l-1$, proves the claim, as $\operatorname{rank} \boldsymbol{U}^{(1)}, \ldots, \operatorname{rank} \boldsymbol{U}^{(l-1)}$ are exactly the minimal possible ranks of an exact QTT decomposition of $\boldsymbol{\sigma}$. □

In Appendix we give a constructive proof of Lemma 12 for $J = 2$, which illustrates the TT approximation algorithm as the sequential low-rank approximation of matrices and results in an explicit low-rank QTT representation of $\boldsymbol{\sigma}$.

Let a function g be Lipschitz continuous on $[-1, 1]$. Consider its Chebyshev projection g_p:

$$g_p = \sum_{k=0}^{p} \alpha_k T_k, \tag{30}$$

where T_k, $k \in \mathbb{Z}_{\geq 0}$, are Chebyshev polynomials of the first kind and

$$\alpha_0 = \frac{1}{\pi} \int_{-1}^{1} \frac{f(x)\, T_0(x)}{\sqrt{1-x^2}} \mathrm{d}x, \quad \alpha_k = \frac{2}{\pi} \int_{-1}^{1} \frac{f(x)\, T_k(x)}{\sqrt{1-x^2}} \mathrm{d}x$$

for $k \in \mathbb{N}$. By our assumptions, the representation $g = \lim_{p\to\infty} g_p$ is unique and absolutely and uniformly convergent. The following proposition relates the decay of the Chebyshev coefficients α_k to the analyticity of g. To formulate it, we denote the open Bernstein ellipse with the parameter $\rho > 1$ by $\mathcal{E}_\rho$:

$$\mathcal{E}_\rho = \left\{ \zeta \in \mathbb{C} : \ \frac{(\Re\zeta)^2}{A^2} + \frac{(\Im\zeta)^2}{B^2} < 1 \right\},$$

where $A = \frac{1}{2}\left(\rho + \rho^{-1}\right)$ and $B = \frac{1}{2}\left(\rho - \rho^{-1}\right)$.

Proposition 13. *Let the function g be analytic in $[-1, 1]$ and admit a holomorphic extension to the open Bernstein ellipse $\mathcal{E}_\rho$ such that $|g(z)| \leq M$ for all $z \in \mathcal{E}_\rho$. Then for each polynomial degree $p \in \mathbb{Z}_{\geq 0}$ the Chebyshev projections g_p in (30) satisfy*

$$\|g - g_p\|_{\mathcal{C}[-1,1]} \leq \frac{2M}{\rho - 1} \rho^{-p} .$$

Proof. See, e.g., Theorem 3.8 in [50] or Theorem 8.2 in [51]. □

In the QTT approximation of polynomials (in particular, of Chebyshev projections) we rely on the following result owing to either of [45, Corollary 13] and [39, Theorem 6].

Proposition 14 (QTT structure of polynomials)**.** *Let $l \in \mathbb{N}$. Assume that a 2^l-component vector $\boldsymbol{p}$ is given by*

$$\boldsymbol{p}_j = \mathcal{P}(j) \quad \text{for} \quad 0 \leq j \leq 2^l - 1,$$

where $\mathcal{P}$ is a univariate polynomial of degree $p \in \mathbb{N}$. Then $\boldsymbol{p}$ has a representation in the QTT format with ranks bounded from above by $p + 1$.

Proposition 15 (Error bound for a tensor product)**.** *Assume $p \in [1, \infty]$. Let $\|\cdot\|$ denote the norms of $\ell_p(\mathcal{I}_k)$, $1 \leq k \leq d$, and of $\ell_p(\mathcal{I}_1 \times \ldots \times \mathcal{I}_d)$, where $\#\mathcal{I}_k = n_k$ for $1 \leq k \leq d$. For $1 \leq k \leq d$, consider vectors $\boldsymbol{p}_k$ and $\tilde{\boldsymbol{p}}_k$ of size n_k, such that*

$$\|\tilde{\boldsymbol{p}}_k - \boldsymbol{p}_k\| \leq \delta_k \|\boldsymbol{p}_k\|$$

for $1 \leq k \leq d$. Then for $\boldsymbol{p} = \boldsymbol{p}_1 \otimes \ldots \otimes \boldsymbol{p}_d$ and $\tilde{\boldsymbol{p}} = \tilde{\boldsymbol{p}}_1 \otimes \ldots \otimes \tilde{\boldsymbol{p}}_d$ with $\delta = \sum_{k=1}^{d} \delta_k$ there holds the estimate

$$\|\tilde{\boldsymbol{p}} - \boldsymbol{p}\| \leq \delta e^{\delta} \|\boldsymbol{p}\| = \left(\delta + \mathcal{O}\left(\delta^2\right)\right) \|\boldsymbol{p}\|, \quad \delta \to 0 .$$

For the proof we refer to the Appendix. □

Proposition 16 (Error bound for a matrix of the CME operator type)**.** *Let $d, R \in \mathbb{N}$, $n_1, \ldots, n_d \in \mathbb{N}$ and $\eta_1, \ldots \eta_s \in \mathbb{Z}^d \setminus \{0\}$. Consider $n_1 \times \ldots \times n_d$-vectors $\boldsymbol{\omega}_1, \ldots, \boldsymbol{\omega}_R \in \mathbb{R}_{\geq 0}^{n_1 \cdot \ldots \cdot n_d}$, $\tilde{\boldsymbol{\omega}}_1, \ldots, \tilde{\boldsymbol{\omega}}_R \in \mathbb{R}^{n_1 \cdot \ldots \cdot n_d}$ and the matrices*

$$\boldsymbol{A} = \sum_{s=1}^{R} (\boldsymbol{S}_{\eta_s} - \mathbb{I}) \cdot \operatorname{diag} \boldsymbol{\omega}_s, \quad \tilde{\boldsymbol{A}} = \sum_{s=1}^{R} (\boldsymbol{S}_{\eta_s} - \mathbb{I}) \cdot \operatorname{diag} \tilde{\boldsymbol{\omega}}_s,$$

where for every $\xi \in \mathbb{Z}^d$ we denote with $\boldsymbol{S}_\xi = \boldsymbol{S}_{1\xi_1} \otimes \ldots \otimes \boldsymbol{S}_{d\xi_d}$ the matrix of a downward ξ-position shift, each factor $\boldsymbol{S}_{k\xi_k}$ being the $n_k \times n_k$-matrix of a downward ξ_k-position shift for $1 \leq k \leq d$.

Consider the following cases:

(a) if $\|\cdot\| = \|\cdot\|_{l_2}$ *and* $\|\cdot\|_\square = \|\cdot\|_{\mathrm{F}}$ *is the Frobenius norm, we denote* $C = \sqrt{R}$*;*

(b) if $\|\cdot\| = \|\cdot\|_{l_\infty}$ *and if* $\|\cdot\|_\square = \|\cdot\|_{\ell_p}$ *is an induced operator norm for* $p \in [1, \infty)$*, we denote* $C = 1$ *and assume additionally that*

$$\left\| \sum_{s=1}^{R} \boldsymbol{\omega}_s \right\| = \sum_{s=1}^{R} \|\boldsymbol{\omega}_s\| \,. \tag{31}$$

Then the estimate

$$\|\tilde{\boldsymbol{\omega}}_s - \boldsymbol{\omega}_s\| \le \delta \, \|\boldsymbol{\omega}_s\|$$

holding for $1 \le s \le R$ *results in the bound*

$$\left\| \tilde{\boldsymbol{A}} - \boldsymbol{A} \right\|_\square \le 2C\delta \, \|\boldsymbol{A}\|_\square \,.$$

For the proof see Appendix. □

The extra assumption (31) of the case (b) of Proposition 16 is satisfied for the propensity vectors corresponding to (11) and (13), since the propensity functions are monotonously increasing.

4 QTT approximation of the CME operator

In the following we consider the FSP of the CME, introduced in Section 2.6, with $n_k = 2^{l_k}$ for $1 \le k \le d$. We consider the operator $\boldsymbol{A}$ given by (6) and truncated to a matrix, in the QTT representation outlined in Section 3.2. In this section we give an upper bound on the QTT ranks of $\boldsymbol{A}$, based on the QTT structure of shift matrices [41, Lemma 3.1], under certain assumptions on the propensity vectors $\{\boldsymbol{\omega}_s\}_{s=1}^R$ defined by (5).

4.1 A general bound

In this section we extend [14, Theorem 2.4] to quantify the error introduced in the CME operator by the approximation of propensity vectors.

Theorem 17. *Under the FSP onto* $\mathcal{Z}_n$ (22)*, consider the CME operator* $\boldsymbol{A}$ *defined by* (6) *. Assume that for every* $s = 1, \ldots, R$ *and* $k = 1, \ldots, d$ *the propensity factor* $\boldsymbol{\omega}_{sk}$ (15) *is approximated in the QTT format by* $\tilde{\boldsymbol{\omega}}_{sk}$ *with relative accuracy* $\frac{\delta}{d\sqrt{R}}$ *and with ranks bounded by* r_{sk}*, where* $\nu_{sk} = \nu'_{sk} = 0$ *implies* $r_{sk} = 1$*. Then the CME operator* $\tilde{\boldsymbol{A}}$ *constructed from the approximate factors of the propensity vectors approximates* $\boldsymbol{A}$ *with relative accuracy* δ *in the Frobenius norm and has a QTT decomposition of ranks*

$$q_1, \ldots, q_1, \hat{q}_1, q_2, \ldots, q_2, \hat{q}_2, \ldots, \ldots, \hat{q}_{d-1}, q_d, \ldots, q_d$$

with $\hat{q}_k = R$ *for* $1 \le k \le d-1$ *and*

$$q_k = \sum_{\substack{s=1,\ldots,R: \\ \nu_{sk}=\nu'_{sk}=0}} 2 \quad + \sum_{\substack{s=1,\ldots,R: \\ \nu_{sk}+\nu'_{sk}\neq 0}} 3\, r_{sk}$$

for $1 \le m_k \le l_k - 1$ *and* $1 \le k \le d$*.*

Proof. The proof follows that of [14, Theorem 2.4] in constructing the CME operator according to formula (6) and using the structure of the Kronecker product, diagonalization, addition and matrix-matrix multiplication in the TT format, presented in Propositions 8–11. The error bounds follow from Propositions 15–16. □

In the theorem above we use the fact that $\nu_{sk} = \nu'_{sk} = 0$ implies that the kth species is not involved in the sth reaction, therefore the one-dimensional factor $\boldsymbol{\omega}_{sk}$ is a vector of ones and $r_{sk} = 1$ is achieved trivially.

The crude upper bound $3Rr$ on the QTT ranks of the CME operator, following from Theorem 17 in terms of $r = \max_{s,k} r_{sk}$, is favourable. Indeed, it ensures the estimate $\mathcal{O}\left(d\, l R^2 r^2\right)$ for the number of parameters, where $l_1, \ldots, l_d \le l$, instead of $\mathcal{O}\left(2^{2ld}\right)$ or $\mathcal{O}\left(2^{ld}\right)$ for the full or sparse elementwise representation respectively.

4.2 QTT approximation of the propensity factors

Next we investigate the QTT structure of the propensity factors $\{\boldsymbol{\omega}_{sk}\}$ (15) corresponding to (9),(10) under the models (12) and (14). In particular, we establish bounds r_{sk} on the QTT ranks of the propensity factors assumed to hold in Theorem 17.

Lemma 18. *Let $l \in \mathbb{N}$, $\nu \in \mathbb{Z} :\ 1 \le \nu < 2^l - 1$. Then the 2^l-component vector $\boldsymbol{u}$ with the entries*

$$\boldsymbol{u}_i = \begin{cases} 0, & 0 \le i < \nu \\ \frac{i!}{(i-\nu)!}, & \nu \le i \le 2^l - 1, \end{cases}$$

can be represented in the QTT format with ranks bounded by $2(\nu + 1)$.

Proof. Define $\boldsymbol{v}_i = (i - \nu + 1) \cdot (i - \nu + 2) \cdot \ldots i$ for $0 \le i \le 2^l - 1$. Then $\boldsymbol{u}$ can be represented through the Hadamard product as follows: $\boldsymbol{u} = \boldsymbol{v} \odot \boldsymbol{\sigma}$, the second factor being considered in Lemma 12 and having a QTT decomposition of ranks bounded by 2. The first factor is composed of the values of a polynomial of degree ν taken on an equidistant mesh. According to Proposition 14, it can be represented in the QTT format with ranks bounded by $\nu+1$. Therefore, by Proposition 8, we obtain the claim. □

Lemma 19. *Let $\upsilon, \nu \in \mathbb{N}$. Assume that $\tau, \mu \in \mathbb{R}$ are such that $\tau \ge 1$ and $\mu > 1$. Consider the function $g : [\nu - 1 + \tau, \nu - 1 + \mu\tau] \to \mathbb{R}$ given by*

$$g(x) = \prod_{j=0}^{\nu-1} \frac{x - j}{\upsilon + x - j} \quad \text{for} \quad x \in [\nu - 1 + \tau, \nu - 1 + \mu\tau]\,. \tag{32}$$

Then for every $p \in \mathbb{N}$ there exists a polynomial $\mathcal{P}$ of degree p such that

$$\|\mathcal{P} - \lambda\|_{\mathcal{C}[\nu-1+\tau, \nu-1+\mu\tau]} \le C\rho^{-p},$$

where $\rho = \frac{\mu + \sqrt{2\mu - 1}}{\mu - 1}$ and $C = 2\frac{1}{\rho - 1} = 2\frac{\mu - 1}{\sqrt{2\mu-1}+1}$.

Proof. Let us extend the function g to $\mathbb{C}$ using the definition (32) for $z \in \mathbb{C}$. The zeros of the nominators on the right-hand side of (32) are simple and located at $\mathcal{N}_1 = \{0, \ldots, \nu - 1\}$; of the denominators, are simple as well and located at $\mathcal{N}_2 = \{-\upsilon, \ldots, -\upsilon + \nu - 1\}$. Hence for $x \ge \nu - 1$ we have $0 \le \frac{x-j}{\upsilon+x-j} < 1$, where $0 \le j \le \nu - 1$, and therefore $|g(x)| \le 1$. If additionally $y \in \mathbb{R}$, then

$$\left| \frac{x + \mathbf{i}y - j}{x + \mathbf{i}y - (j - \upsilon)} \right| \le 1,$$

and for $\Re z \ge \nu - 1$ we have the bound $|g(z)| \le 1$.

Let us define $m = \nu - 1 + \frac{\mu\tau + \tau}{2} = \nu - 1 + \tau\frac{\mu+1}{2}$ and $f = \frac{\mu\tau - \tau}{2} = \tau\frac{\mu-1}{2}$. Then g is analytic in the ellipse

$$E = \left\{ z \in \mathbb{C} :\ \frac{(\Re z - m)^2}{a^2} + \frac{(\Im z)^2}{b^2} < 1 \right\},$$

where $a = f + \tau = \tau\frac{\mu}{2}$ and $b = \sqrt{a^2 - f^2} = \tau\frac{\sqrt{2\mu-1}}{2}$, with the foci $m - f = \nu - 1 + \tau$ and $m + f = \nu - 1 + \mu\tau$.

Consider the affine mapping $\varphi : \mathbb{C} \to \mathbb{C}$ given by $\varphi(\zeta) = m + f \cdot \zeta$ for $\zeta \in \mathbb{C}$, so that $\varphi[-1,1] = [\nu - 1 + \tau, \nu - 1 + \mu\tau]$ and $\varphi^{-1}(z) = -1 - 2\frac{\nu-1+\tau-z}{(\mu-1)\tau}$ for all $z \in \mathbb{C}$. Then the function $G = g \circ \varphi : \mathbb{C} \to \mathbb{C}$ is analytic and satisfies

$$|G(\zeta)| = |g(x + \mathbf{i}y)| \leq 1$$

at every point ζ of the open Bernstein ellipse $\mathcal{E}_\rho = \varphi^{-1}E$ with $\rho = 2\frac{a+b}{(\mu-1)\tau} = \frac{\mu+\sqrt{2\mu-1}}{\mu-1}$, where we denote $x = \Re\,\varphi(\zeta)$ and $y = \Im\,\varphi(\zeta)$. By Proposition 13, for G_p chosen as the pth Chebyshev projection of G we have the estimate $\|G - G_p\|_{\mathcal{C}[-1,1]} \leq \frac{2}{\rho-1}\rho^{-p} = C\rho^{-p}$. Then for $\mathcal{P} = G_p \circ \varphi^{-1}$, which is a polynomial of degree p, we have $\|g - \mathcal{P}\|_{\mathcal{C}[\nu-1+\tau,\nu-1+\mu\tau]} = \|G - G_p\|_{\mathcal{C}[-1,1]}$.

□

Theorem 20. *Let $\upsilon, \nu, l \in \mathbb{N} :\ 1 \leq \upsilon, \nu < 2^l - 1$. Consider the 2^l-component vector $\boldsymbol{u}$ given by*

$$\boldsymbol{u}_i = \begin{cases} 0, & 0 \leq i < \nu, \\ g(i)\,, & \nu \leq i < 2^l, \end{cases}$$

generated by a function g defined by

$$g(x) = \prod_{j=0}^{\nu-1} \frac{x - j}{\upsilon + x - j} \quad \textit{for} \quad x \in \left[\nu, \nu + 2^l - 1\right].$$

Then for any real $p \geq 1$ there exists a 2^l-component vector $\boldsymbol{v}$ which can be exactly represented in the QTT format with ranks bounded by

$$r = 3\,l\,(p+2) + 3\,\frac{(l-1)\,l}{\log_2 \rho},$$

and such that

$$\|\boldsymbol{v} - \boldsymbol{u}\|_{\ell_2} \leq \sqrt{2}\,C\rho^{-p},$$

where $\rho = 2 + \sqrt{3}$ and $C = \frac{2}{1+\sqrt{3}}$.

Proof. Let us define $\tau_k = \nu - 1 + 2^k$ for $0 \leq k \leq l$ and $p_k = \lceil p + \beta\,(k-1) \rceil$ for $1 \leq k \leq l$, where $\beta > 0$ is to be specified below. By Lemma 19, for $1 \leq k \leq l$ there exists a polynomial $\mathcal{P}_k$ of degree p_k such that

$$\|\mathcal{P}_k - g\|_{\mathcal{C}[\tau_{k-1},\tau_k]} \leq C\rho^{-p_k}.$$

For $1 \leq k \leq l$ we define 2^l-component vectors $\boldsymbol{\sigma}_k$ and $\boldsymbol{v}_k$ as follows:

$$\boldsymbol{\sigma}_{ki} = \begin{cases} 0, & 0 \leq i < \tau_{k-1}, \\ 1, & \tau_{k-1} \leq i < \tau_k, \\ 0, & \tau_k \leq i < 2^l \end{cases}$$

and

$$\boldsymbol{v}_{ki} = \mathcal{P}_k(i)\,, \quad 0 \leq i < 2^l. \tag{33}$$

Then the error of the approximation of $\boldsymbol{u} = \sum_{k=1}^{l} \boldsymbol{u} \odot \boldsymbol{\sigma}_k$ by $\boldsymbol{v} = \sum_{k=1}^{l} \boldsymbol{v}_k \odot \boldsymbol{\sigma}_k$ satisfies

$$\begin{aligned} \|\boldsymbol{v} - \boldsymbol{u}\|_{\ell_2}^2 &= \sum_{k=1}^{l} \|(\boldsymbol{v}_k - \boldsymbol{u}) \odot \boldsymbol{\sigma}_k\|_{\ell_2}^2 \leq \sum_{k=1}^{l} 2^{k-1}\,\|\mathcal{P}_k - g\|_{\mathcal{C}[\tau_{k-1},\tau_k]}^2 \\ &\leq C^2 \sum_{k=1}^{l} 2^{k-1}\rho^{-2p_k} \leq C^2\rho^{-2p} \sum_{k=0}^{l-1} 2^k \rho^{-2\beta k} \leq 2\,C^2\rho^{-2p}, \end{aligned}$$

where we defined $\beta = \log_2^{-1} \rho$.

By Proposition 14, for $1 \le k \le l$ the vector $\boldsymbol{v}_k$ defined by (33) can be exactly represented in the QTT format with ranks bounded by $p_k + 1$ uniformly in l. On the other hand, Lemma 12 bounds the QTT ranks of $\boldsymbol{\sigma}_k$ by 3. Therefore, by [31, Section 4], we obtain the upper bound r on the ranks of an exact QTT representation of $\boldsymbol{v}$:

$$\sum_{k=1}^{l} 3p_k = 3\sum_{k=0}^{l-1} \left(\lceil p + \beta k \rceil + 1\right) \le 3l\,(p+2) + 3\beta\,(l-1)\,l = r,$$

which completes the proof. □

4.3 Rank bound for the particular kinetics

The preceding Theorem 20 shows that under the Michaelis–Menten kinetics the kth factor of the propensity vector (15) corresponding to the sth reaction can be approximated in the QTT format with accuracy ε_{sk} in the ℓ_2-norm and with QTT ranks

$$r_{sk} = \mathcal{O}\left(\log \frac{1}{\varepsilon_{sk}} \cdot \log n_k\right) + \mathcal{O}\left(\log^2 n_k\right),$$

where $n_k = 2^{l_k}$ is the bound on the copy number in the Finite State Projection for the kth species. As the propensity function tends to 1 for large arguments, the norm of the kth factor of the propensity vector (15) can be estimated as $\|\boldsymbol{\omega}_{sk}\|_{\ell_2} = \mathcal{O}\left(n_k^{1/2}\right)$, $n_k \to \infty$. For example, note that $\boldsymbol{\omega}_{sk\,i_k} \ge \frac{1}{2}$ for $i_k \ge (\nu_{sk} - 1) + \upsilon_k\,(2\nu_{sk} - 1)$. Given $\delta > 0$, we set

$$\varepsilon_{sk} = \frac{\delta}{2d\sqrt{R}} \|\boldsymbol{\omega}_{sk}\|, \tag{34}$$

so that, by Theorem 20, for $1 \le k \le d$ and $1 \le s \le R$ there exists a QTT approximation of the propensity factor $\boldsymbol{\omega}_{sk}$ with accuracy ε_{sk} in the ℓ_2-norm and with QTT ranks bounded by

$$r = \mathcal{O}\left(\left(\log \frac{1}{\delta} + \log d + \log R + \log n\right) \log n\right),$$

where $n \ge n_1, \ldots, n_d$. Then, by Theorem 17, the truncated CME operator $\tilde{\boldsymbol{A}}$ constructed from such approximations, in turn, approximates with relative accuracy δ in the Frobenius norm the truncated CME operator $\boldsymbol{A}$ constructed from exact propensity factors. The approximation is constructed in the QTT format with ranks bounded by

$$3Rr = \mathcal{O}\left(R\left(\log \frac{1}{\delta} + \log d + \log R + \log n\right) \log n\right). \tag{35}$$

If the kth species reacts under the mass-action kinetics, by Lemma (18), we obtain the bound

$$3Rr = 3R\,(\nu + 1) \tag{36}$$

on the corresponding $l_k - 1$ QTT ranks, where $\nu \ge \nu_{sk}$, $1 \le s \le R$. The bound (36) is independent of n, d and of the accuracy δ. In principle, the factor d in (34)–(35) can be reduced then.

The estimate (35) is almost linear in R (up to a logarithmic factor), logarithmic in n, d and δ. In view of (29), the bound (35) implies that the CME operator for the Michaelis–Menten kinetics, considered under the FSP outlined in Section 2.6, can be approximated in the QTT format with relative accuracy δ in the Frobenius norm with the storage cost being almost linear in d (up to a logarithmic factor), almost quadratic in R (up to a logarithmic factor) and logarithmic in n and δ. In the case of the mass-action kinetics, the estimate is linear in d, logarithmic in n and quadratic in the upper bound on $\{\nu_k\}$. For mixed kinetics the maximum of the two asymptotics should be considered. Analogous conclusions follow from (35)–(36) for the complexity of basic linear algebra operations with the CME operator in the QTT format.

5 QTT approximation of stationary distributions of CRNs

We now turn to the QTT approximation of FSP truncations of the invariant distribution given by Theorem 5. The distribution is separable, i.e. of TT ranks $1, \ldots, 1$. As a result, QTT approximations of the full PDF (5) can be constructed as the Kronecker product of QTT approximations of the factors. Since the factors are evaluations of analytic functions on equidistant grids in the spaces of copy numbers, bounds on the QTT ranks of approximations, logarithmic in the accuracy parameter ε, can be expected. In the present section, we aim at obtaining bounds which reveal also the dependence of the QTT ranks on the propensity parameters of the kinetics models and of the maximal copy numbers allowed by the FSP truncation.

5.1 QTT approximation of propensity factors

Lemma 21. *Let $\lambda > 0$ and consider the function g given by*

$$g(x) = \frac{\lambda^x}{\Gamma(x+1)} \quad \text{for all real} \quad x > 0.$$

For $\mu > 1$ denote

$$\alpha = \pi \left(\sqrt{\frac{\mu}{2\mu+1}} - \frac{1}{2} \right).$$

Then for every $\tau \in \mathbb{R}$: $\tau \geq 1$ and $\tau \geq 2e^{\alpha}\lambda$ and for every $p \in \mathbb{N}$ there exists a polynomial $\mathcal{P}$ of degree p such that

$$\|\mathcal{P} - g\|_{\mathcal{C}[\tau, \mu\tau]} \leq \frac{2MC}{\rho - 1} \rho^{-p},$$

where the constants are explicitly given by

$$C = \frac{e^{\alpha}}{\sqrt{1 - e^{-3\pi}}\sqrt{\pi}} \left(\frac{\mu}{2\mu+1} \right)^{\frac{1}{4}}, \quad M = \frac{e^{(\alpha+1+\log\lambda)\tau}}{\tau^{\tau+\frac{1}{2}}}, \quad \rho = \frac{\mu + \sqrt{2\mu - 1}}{\mu - 1}.$$

Proof. The function g extended to the whole complex plane by

$$g(z) = \frac{\lambda^z}{\Gamma(z+1)}, \quad z \in \mathbb{C},$$

is entire, since the exponential and reciprocal Gamma functions are so. Let us define $\delta = \frac{\tau}{2}$, $m = \frac{\mu\tau+\tau}{2} = \tau\frac{\mu+1}{2}$ and $f = \frac{\mu\tau-\tau}{2} = \tau\frac{\mu-1}{2}$. Then the Bernstein ellipse

$$E = \left\{ z \in \mathbb{C} : \ \frac{(\Re z - m)^2}{a^2} + \frac{(\Im z)^2}{b^2} < 1 \right\},$$

where $a = f + \delta = \tau\frac{\mu}{2}$ and $b = \sqrt{a^2 - f^2} = \tau\frac{\sqrt{2\mu-1}}{2}$, has foci $m - f = \tau$ and $m + f = \mu\tau$. Moreover, E is enclosed between the two tangents to its boundary that are given by $\Im z = \pm\phi\Re z$ with $\phi = \frac{b}{\sqrt{m^2-a^2}} = \sqrt{\frac{2\mu-1}{2\mu+1}}$.

By [52, 6.1.25], for all $\xi > 0$ and $y \in \mathbb{R}$ we have

$$\left| \frac{\Gamma(\xi)}{\Gamma(\xi + \mathbf{i}y)} \right|^2 = \prod_{n=0}^{\infty} \left(1 + \frac{y^2}{(\xi+n)^2} \right)$$

We may bound this infinite product as follows:

$$\left| \frac{\Gamma(\xi)}{\Gamma(\xi + \mathbf{i}y)} \right|^2 \leq \left(1 + \frac{y^2}{\xi^2} \right) \prod_{n=1}^{\infty} \left(1 + \frac{y^2}{\xi^2 + n^2} \right).$$

The infinite product written in the right-hand side reads

$$\prod_{n=1}^{\infty}\left(1+\frac{y^2}{\xi^2+n^2}\right)=\prod_{n=1}^{\infty}\frac{\xi^2+n^2+y^2}{\xi^2+n^2}=\prod_{n=1}^{\infty}\frac{\xi^2+n^2+y^2}{n^2}\frac{n^2}{\xi^2+n^2}$$
$$=\frac{\prod_{n=1}^{\infty}\left(1+\frac{\xi^2+y^2}{n^2}\right)}{\prod_{n=1}^{\infty}\left(1+\frac{\xi^2}{n^2}\right)}=\frac{\frac{1}{\pi\sqrt{\xi^2+y^2}}\sinh\pi\sqrt{\xi^2+y^2}}{\frac{1}{\pi\xi}\sinh\pi\xi},$$

where at the last step we used the Weierstraß factorization [52, 4.5.68] for $z\mapsto\frac{\sinh z}{z}$. Therefore, provided that $|y|\le\psi\,\xi$ with some $\psi>0$, we have

$$\left|\frac{\Gamma(\xi)}{\Gamma(\xi+\mathbf{i}y)}\right|^2\le\sqrt{1+\psi^2}\,\frac{1}{1-e^{-2\pi\xi}}\,e^{\pi\xi\left(\sqrt{1+\psi^2}-1\right)}. \tag{37}$$

On the other hand, by [52, 6.1.38], for all $x>0$ it holds that

$$\Gamma(x+1)\ge\sqrt{2\pi}\,x^{x+\frac{1}{2}}\,e^{-x}. \tag{38}$$

For every point $x+\mathbf{i}y\in E$, where $x,y\in\mathbb{R}$, the bounds $x\ge m-a=\frac{1}{2}\tau$ and $|y|\le\phi x$ are satisfied, therefore $x+1\ge1+\frac{1}{2}\tau\ge\frac{3}{2}$ and $|y|\le\phi\,(x+1)$. Then the bounds (37) and (38) yield the estimate

$$|g(x+\mathbf{i}y)|\le C\,\frac{e^{(\alpha+1+\log\lambda)x}}{x^{x+\frac{1}{2}}}\le CM,$$

where $\alpha=\frac{\pi}{2}\left(\sqrt{1+\phi^2}-1\right)=\pi\left(\sqrt{\frac{\mu}{2\mu+1}}-\frac{1}{2}\right)$ and $C=\frac{\left(1+\phi^2\right)^{\frac{1}{4}}}{\sqrt{1-e^{-3\pi}}\sqrt{2\pi}}\,e^{\alpha}=\left(\frac{4\mu}{2\mu+1}\right)^{\frac{1}{4}}\frac{e^{\alpha}}{\sqrt{1-e^{-3\pi}}\sqrt{2\pi}}$, and the last step uses that, by assumption, $x\ge\frac{\tau}{2}\ge e^{\alpha}\lambda$ and hence the bound monotonically decreases with respect to x.

Consider the affine mapping $\varphi:\mathbb{C}\to\mathbb{C}$ given by $\varphi(\zeta)=m+f\cdot\zeta$ for $\zeta\in\mathbb{C}$, so that $\varphi\,[-1,1]=[\tau,\mu\tau]$ and $\varphi^{-1}(z)=-1-2\frac{\tau-z}{(\mu-1)\tau}$ for all $z\in\mathbb{C}$. Then the function $G=g\circ\varphi:\mathbb{C}\to\mathbb{C}$ is entire and satisfies

$$|G(\zeta)|=|g(x+\mathbf{i}y)|\le CM$$

at every point ζ of the open Bernstein ellipse $\mathcal{E}_\rho=\varphi^{-1}E$ with $\rho=2\frac{a+b}{(\mu-1)\tau}=\frac{\mu+\sqrt{2\mu-1}}{\mu-1}$, where we denote $x=\Re\,\varphi(\zeta)$ and $y=\Im\,\varphi(\zeta)$. By Proposition 13, for G_p chosen as the pth Chebyshev projection of G and for $\mathcal{P}=G_p\circ\varphi^{-1}$, which is also a polynomial of degree p, we obtain

$$\|g-\mathcal{P}\|_{\mathcal{C}[\tau,\mu\tau]}=\|G-G_p\|_{\mathcal{C}[-1,1]}\le\frac{2\,CM}{\rho-1}\rho^{-p}.$$

□

Theorem 22. *Assume $\lambda>0$ and $l\in\mathbb{N}$ are such that $1\le2e^{\alpha}\lambda<2^l-1$, where $\alpha=\pi\left(\sqrt{\frac{2}{5}}-\frac{1}{2}\right)$. Consider the 2^l-component vector $\boldsymbol{u}$ given by*

$$\boldsymbol{u}_i=g(i)\quad\text{for}\quad0\le i<2^l,$$

generated by the function $g(x)=\lambda^x/\Gamma(x+1)$ for $0<x\in\mathbb{R}$. Suppose $\varepsilon>0$ and $K_\infty\in\mathbb{N}$ are such that

$$K_\infty\ \ge\ \log_2 2e\lambda, \tag{39}$$
$$K_\infty\ \ge\ \log_2\left(2\log_2\frac{1}{\varepsilon}+1-\log_2\pi\right)-1, \tag{40}$$

and set $K_l=\min\{K_\infty,l\}$.

Then there exists a 2^l-component vector $\boldsymbol{v}$ which satisfies $\|\boldsymbol{v}-\boldsymbol{u}\|_{\ell_2}\le\varepsilon$ and can be exactly represented in the QTT format with ranks bounded from above by

$$r = r_0 + 3\,(K_l - k_0)\left(2 + \log_\rho \frac{2C_1}{\varepsilon}\right) + \frac{3}{4\beta}\,(K_l - k_0 - 1)\,(K_l - k_0)\,,$$

where $r_0 = 2\sqrt{e^{\alpha+1}\lambda}$, $k_0 = \lceil \log_2 e^{\alpha+1}\lambda \rceil$ and the constants are given explicitly by

$$C_1 = \frac{2\,C}{\rho - 1}, \quad C = \frac{e^\alpha}{\sqrt{1-e^{-3\pi}}\sqrt{\pi}}\left(\frac{2}{5}\right)^{\frac{1}{4}}, \quad \beta = \log_2\rho, \quad \rho = 2+\sqrt{3}\,.$$

Proof. First we note that $2^{k_0} \ge e^{\alpha+1}\lambda$. For $k_0 \le k \le l$ we define $\tau_k = 2^k$ and for $k_0+1 \le k \le l$ introduce a 2^l-component vector $\boldsymbol{\sigma}_k$ as follows:

$$\boldsymbol{\sigma}_{ki} = \begin{cases} 0, & 0 \le i < \tau_{k-1}, \\ 1, & \tau_{k-1} \le i < \tau_k, \\ 0, & \tau_k \le i < 2^l. \end{cases}$$

Using the estimate (38), for $K_\infty < k \le l$ we obtain

$$\begin{aligned}\|\boldsymbol{u}\odot\boldsymbol{\sigma}_k\|_{\ell_2}^2 &\le 2^{k-1}\,\|g\|_{\mathcal{C}[\tau_{k-1},\tau_k]}^2 \le 2^{k-1}\,\frac{1}{2\pi}\frac{e^{2\tau_{k-1}}\lambda^{2\tau_{k-1}}}{\tau_{k-1}^{2\tau_{k-1}+1}} \\ &= \frac{1}{2\pi}\,e^{2^k(1+\log\lambda-(k-1)\log 2)} = \frac{1}{2\pi}\,2^{2^k(\gamma-k)},\end{aligned}$$

where we denote $\gamma = 1 + \log_2 e + \log_2\lambda$. Then

$$\begin{aligned}&\sum_{k=K_l+1}^{l}\|\boldsymbol{u}\odot\boldsymbol{\sigma}_k\|_{\ell_2}^2 \le \sum_{k=K_\infty+1}^{\infty}\|\boldsymbol{u}\odot\boldsymbol{\sigma}_k\|_{\ell_2}^2 \le \frac{1}{2\pi}\sum_{k=K_\infty+1}^{\infty}2^{-2^{K_\infty+1}(k-\gamma)} \\ &\le \frac{1}{2\pi}2^{-2^{K_\infty+1}(K_\infty+1-\gamma)}\frac{1}{1-2^{-4}} \le \frac{1}{\pi}2^{-2^{K_\infty+1}(K_\infty+1-\gamma)} \le \frac{1}{\pi}2^{-2^{K_\infty+1}},\end{aligned}$$

where for the last step we refer to (39). By taking into account the condition (40), we conclude that

$$\sum_{k=K_l+1}^{l}\|\boldsymbol{u}\odot\boldsymbol{\sigma}_k\|_{\ell_2}^2 \le \frac{\varepsilon^2}{2}\,. \tag{41}$$

Let us now assume $k_0+1 \le k \le K_l$. By Lemma 21, for $k_0+1 \le k \le K_l$ there exists a polynomial $\mathcal{P}_k$ of degree

$$p_k = \left\lceil \frac{1}{\beta}\left(\log_2\frac{2C_1}{\varepsilon} + \frac{k-k_0-1}{2}\right)\right\rceil, \tag{42}$$

such that

$$\|\mathcal{P}_k - g\|_{\mathcal{C}[\tau_{k-1},\tau_k]} \le C_1 M_k\,\rho^{-p_k},$$

where $M_k = \frac{e^{(\alpha+1)\tau_{k-1}}\lambda^{\tau_{k-1}}}{\tau_{k-1}^{\tau_{k-1}+\frac{1}{2}}} = \frac{e^{(\alpha+1+\log\lambda)2^{k-1}}}{2^{(k-1)\left(2^{k-1}+\frac{1}{2}\right)}}$. Let us evaluate $\mathcal{P}_k$ at the integer points of $\big[0, 2^l-1\big]$: to this end, we define a 2^l-component vector $\boldsymbol{v}_k$ with entries

$$(\boldsymbol{v}_k)_{\,i} = \lambda^i\cdot\mathcal{P}_k(i)\,, \quad 0 \le i < 2^l\,. \tag{43}$$

Having done that for $k_0+1 \le k \le K_l$, let us denote $\boldsymbol{u}_0 = \boldsymbol{u} - \sum_{k=k_0+1}^{l}\boldsymbol{u}\odot\boldsymbol{\sigma}_k$. Then the error $\boldsymbol{v}-\boldsymbol{u}$ of the approximation of $\boldsymbol{u} = \boldsymbol{u}_0 + \sum_{k=k_0+1}^{l}\boldsymbol{u}\odot\boldsymbol{\sigma}_k$ by

$$\boldsymbol{v} = \boldsymbol{u}_0 + \sum_{k=k_0+1}^{K_l}\boldsymbol{v}_k\odot\boldsymbol{\sigma}_k \tag{44}$$

satisfies the bound

$$\|(\boldsymbol{v}-\boldsymbol{u})\odot\boldsymbol{\sigma}_k\|_{\ell_2}^2 \le 2^{k-1}\,\|\mathcal{P}_k-g\|_{\mathcal{C}[\tau_{k-1},\tau_k]}^2$$
$$\le 2^{k-1}C_1^2\rho^{-2p_k}\frac{e^{(\alpha+1+\log\lambda)2^k}}{2^{(k-1)(2^k+1)}} = C_1^2\rho^{-2p_k}\;2^{-2\beta p_k+2^k(\gamma'-k)} \le 2^{-2\beta p_k}, \tag{45}$$

where $\gamma' = \gamma+\alpha\log_2 e = 1+(1+\alpha)\log_2 e+\log_2\lambda \le k_0+1 \le k+1$, for $k_0+1\le k\le K_l$. Consequently, for the error of the approximation on $[\tau_{k_0},\tau_{K_l}]$ we obtain the bound

$$\sum_{k=k_0+1}^{K_l}\|(\boldsymbol{v}-\boldsymbol{u})\odot\boldsymbol{\sigma}_k\|_{\ell_2}^2 \le \frac{\varepsilon^2}{4}\sum_{k=0}^{\infty}2^{-k} = \frac{\varepsilon^2}{2},$$

which together with (41) yields $\|\boldsymbol{v}-\boldsymbol{u}\|_{\ell_2}\le\varepsilon$.

Finally, due to the structure of the addition and Hadamard multiplication in the TT format, presented in Proposition 8, the upper bound r on the ranks of an exact QTT representation of $\boldsymbol{v}$ can be obtained as follows: the first term $\boldsymbol{u}_0$ in the right-hand side of (44) is nonzero only in the leading 2^{k_0}-component subvector. Therefore the rank of each of its unfolding matrices is bounded by

$$2^{\left\lceil\frac{k_0-1}{2}\right\rceil} \le 2^{\frac{k_0+1}{2}} \le 2\sqrt{e^{\alpha+1}\lambda} = r_0,$$

and $\boldsymbol{u}_0$ can be represented in the QTT format with ranks bounded by r_0. By Proposition 14, for $k_0+1\le k\le K_l$ the vector $\boldsymbol{v}_k$ defined by (43) can be exactly represented in the QTT format with ranks bounded by p_k+1. On the other hand, Lemma 12 bounds the QTT ranks of $\boldsymbol{\sigma}_k$ by 3. Thus, we estimate the QTT ranks of $\boldsymbol{v}$ from above by

$$r_0+\sum_{k=k_0+1}^{K_l}3\,(p_k+1) \le r_0+3\,(K_l-k_0)\left(2+\log_\rho\frac{2C_1}{\varepsilon}\right)$$
$$+\frac{3}{4\beta}\,(K_l-k_0-1)\,(K_l-k_0) = r,$$

which concludes the proof. □

Remark 23. *Due to the rapid decay with respect to k of the function considered in Lemma 21 and of the approximation error, both being considered on the kth interval, the polynomial degree of the approximant does not need to grow linearly with respect to k, as we require in* (42)*. Indeed, the last step of* (45) *for the sake of simplicity neglects a very rapidly decaying factor and therefore could be replaced with a sharper estimate. As a result, for large l and small ε the rank bound of Theorem 22 could be refined from quadratic to linear with respect to K_l-k_0.*

Lemma 24. *Let $\vartheta,\lambda>0$ and $\upsilon,l\in\mathbb{N}$. Then the 2^l-component vector $\boldsymbol{u}$ with the entries*

$$\boldsymbol{u}_i = \frac{\lambda^i}{\prod_{j=1}^i\theta(j)},\quad 0\le i<2^l,$$

where

$$\theta(x) = \frac{\vartheta x}{\upsilon+x}\quad \textit{for all}\quad x>0,$$

can be represented in the QTT format with ranks bounded by $\upsilon+1$.

Proof. For all i we have

$$\boldsymbol{u}_i = \frac{\lambda^i}{\prod_{j=1}^i\theta(j)} = \left(\frac{\lambda}{\vartheta}\right)^i\frac{\prod_{j=1}^i(\upsilon+j)}{\prod_{j=1}^i j} = \left(\frac{\lambda}{\vartheta}\right)^i\frac{1}{\upsilon!}\frac{(\upsilon+i)!}{i!}$$
$$= \left(\frac{\lambda}{\vartheta}\right)^i\frac{1}{\upsilon!}\,(i+1)\cdot(i+2)\cdot\ldots\cdot(i+\upsilon),$$

that is $\boldsymbol{u} = \boldsymbol{w} \odot \boldsymbol{v}$, where $\boldsymbol{w}_i = \left(\frac{\lambda}{\vartheta}\right)^i$ and $\boldsymbol{v}_i = \frac{1}{\upsilon!}(i+1)\cdot(i+2)\cdot\ldots\cdot(i+\upsilon)$ for $0 \le i < 2^l$. By Proposition 14, the vector $\boldsymbol{v}$ which consists of the values of a polynomial of degree at most υ evaluated on an equidistant mesh can be exactly represented in the QTT format with ranks bounded by $\upsilon + 1$. The first factor has an exact rank-one representation, see Example 7. Then the claim follows due to Proposition 8. □

5.2 Approximation of distributions

It follows from Theorem 22 that under the mass-action kinetics the kth factor $\boldsymbol{p}_k$ (21) of the stationary distribution $\boldsymbol{p}$ (20) upon the FSP can be approximated with a given absolute accuracy ε_k in the ℓ_2-norm in the QTT format with ranks bounded by

$$r_k = \mathcal{O}\left(c_k^{\frac{1}{2}}\right) + \mathcal{O}\left(\log\frac{1}{\varepsilon_k}\ \cdot\ \log n_k\right) + \mathcal{O}\left(\log^2 n_k\right), \tag{46}$$

and, for large n_k, by

$$r_k = \mathcal{O}\left(c_k^{\frac{1}{2}}\right) + \mathcal{O}\left(\left(\log\frac{1}{\varepsilon_k}\right)\cdot\log\log\frac{1}{\varepsilon_k}\right), \tag{47}$$

where $n_k = 2^{l_k}$ is the bound on the copy number in the FSP for the kth species and λ_k is the parameter of the corresponding Poisson distribution. As for the Michaelis–Menten kinetics, Lemma 24 gives the bound $\upsilon_k + 1$ on the ranks of an exact QTT representation of the kth factor given by (21). Given $\varepsilon > 0$, we may set the accuracy

$$\varepsilon_k = \frac{\varepsilon}{d}\frac{\|\boldsymbol{p}\|_{\ell_2}}{\|\boldsymbol{p}_k\|_{\ell_2}} = \frac{\varepsilon}{d}\prod_{k'\neq k}\|\boldsymbol{p}_{k'}\|_{\ell_2} \tag{48}$$

for the approximation of the kth factor, $1 \le k \le d$. This, by Proposition 15, ensures that the tensor product of such approximations, in turn, approximates the distribution with accuracy ε in the ℓ_2-norm. Since for all reasonably large FSP truncations the norms $\|\boldsymbol{p}_k\|$, $1 \le k \le d$, are close to the upper bounds they take when no FSP is employed, for a particular distribution the QTT ranks of the resulting approximation are bounded from above by

$$r = \mathcal{O}\left(c^{\frac{1}{2}}\right) + \mathcal{O}\left(\log\frac{d}{\varepsilon}\ \cdot\ \log n\right) + \mathcal{O}\left(\log^2 n\right), \tag{49}$$

where $n \ge n_1, \ldots, n_d$ and $c \ge c_1, \ldots, c_d$, and, for large n, by

$$r = \mathcal{O}\left(c^{\frac{1}{2}}\right) + \mathcal{O}\left(\left(\log\frac{d}{\varepsilon}\right)\cdot\log\log\frac{d}{\varepsilon}\right)\ . \tag{50}$$

If the kth species reacts under the Michaelis–Menten kinetics, we have the bound on the corresponding $l_k - 1$ QTT ranks that reads instead as

$$r_k = \upsilon_k + 1 \tag{51}$$

independently of the accuracy ε and, in principle, the factor d in (48)–(50) can be reduced.

In view of the estimate (29), the bounds (49)–(51) imply that the stationary distribution given by (20)-(21) for the mass-action kinetics, considered under the FSP outlined in Section 2.6, can be approximated in the QTT format with accuracy ε with the storage cost being almost linear in d (up to a logarithmic factor) and logarithmic in ε. For moderate n it is also logarithmic in n and, for large n, it is independent of n. In the case of the Michaelis–Menten kinetics, our rank bound is linear in d, logarithmic in n and quadratic in the upper bound on the corresponding parameters $\{\upsilon_k\}$. For mixed kinetics the maximum of the two asymptotics should be considered. Similar conclusions result from (49)–(51) for the complexity of basic linear algebra operations with the the stationary distributions in the QTT format.

Remark 25. *The result of Theorem 22 can be refined for large λ: indeed, in the proof a piecewise-polynomial approximation, similar to what we use on $[2^{k_0}, 2^{K_l}]$, could be constructed and represented in the QTT format on $[0, 2^{k_0}]$, where we currently decompose the distribution in the QTT representation without any compression. This would allow to relax the dependence on λ in Theorem 22; and on c_k and c, in the consequent bounds* (46)–(50).

6 Conclusion

In the case of mass-action, Michaelis–Menten or mixed kinetics, we presented a rank-accuracy analysis for the QTT-formatted representation of the CME operator (Section 4.3). We showed that for a desired relative accuracy ε in the Frobenius norm that one can construct a QTT representation of the CME operator with the number of parameters logarithmic with respect to the maximum copy number and the accuracy, quadratic with respect to the number of reactions and almost linear (up to a logarithmic factor) with respect to the number of reacting species. When all species follow the mass-action kinetics law, the propensities are polynomial, and for any accuracy the operator can be represented exactly with uniformly low ranks.

Also, we considered a stationary distribution for a stochastic model with a weakly reversible reaction network and zero deficiency in the sense of Feinberg, given by Theorem 5 [16, Theorem 6.1]. We showed for the two kinetics models mentioned above that the stationary distribution can be approximated in the QTT format with any prescribed accuracy in the ℓ_2-norm and with low ranks. The bound on the number of parameters involved is almost linear in the number of reacting species (up to a logarithmic factor) and logarithmic in both the maximum copy number and accuracy. When all species obey the Michaelis–Menten kinetics law, the estimate is independent of the accuracy.

The problems for the CME that may require tensor approximations are so large that even under the FSP the norms, which are equivalent theoretically, may differ significantly in practice. In the present paper we use the ℓ_2- and Frobenius norms for the approximation of distributions and of the CME operator respectively. This choice is conditioned by the current state of the art of efficient and robust algorithms for the approximation and truncation in the TT and QTT formats, which are presently available only for the mentioned norms. The results of this paper justify the low-rank structure observed with the use of such algorithms, see [14]. However, we would like to emphasize that the natural choice of the norms would be different due to the probabilistic sense of the data involved in the problem, and the theoretical analysis of this paper can be adapted to other norms. In particular, the approximations constructed in Theorems 20 and 22 can be easily modified to satisfy analogous error bounds in the ℓ_1- or ℓ_∞-norms.

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Appendix

Proofs of Propositions 15 and 16

Proof of Proposition 15. By the triangle inequality,

$$\begin{aligned}\|\tilde{\boldsymbol{p}}-\boldsymbol{p}\| &\le \sum_{k=1}^{d}\left\|\tilde{\boldsymbol{p}}_1\otimes\ldots\otimes\tilde{\boldsymbol{p}}_{k-1}\otimes(\tilde{\boldsymbol{p}}_k-\boldsymbol{p}_k)\otimes\boldsymbol{p}_{k+1}\otimes\ldots\otimes\boldsymbol{p}_d\right\|,\\ &\le \|\boldsymbol{p}\|\sum_{k=1}^{d}\delta_k\,\frac{\|\tilde{\boldsymbol{p}}_1\|}{\|\boldsymbol{p}_1\|}\cdots\frac{\left\|\tilde{\boldsymbol{p}}_{k-1}\right\|}{\left\|\boldsymbol{p}_{k-1}\right\|}\le\|\boldsymbol{p}\|\sum_{k=1}^{d}\delta_k\;(1+\delta_1)\cdots(1+\delta_{k-1})\\ &\le \|\boldsymbol{p}\|\sum_{k=1}^{d}\delta_k\;\exp\left(\sum_{k=1}^{d}\delta_k\right).\end{aligned}$$

□

Proof of Proposition 16. By the triangle inequality we obtain

$$\begin{aligned}\left\|\tilde{\boldsymbol{A}}-\boldsymbol{A}\right\|_{\square} &\le \sum_{s=1}^{R}\|(\boldsymbol{S}_{\eta_s}-\mathbb{I})\cdot\operatorname{diag}(\tilde{\boldsymbol{\omega}}_s-\boldsymbol{\omega}_s)\|_{\square}\\ &\le \sum_{s=1}^{R}\|\boldsymbol{S}_{\eta_s}\operatorname{diag}(\tilde{\boldsymbol{\omega}}_s-\boldsymbol{\omega}_s)\|_{\square}+\sum_{s=1}^{R}\|\operatorname{diag}(\tilde{\boldsymbol{\omega}}_s-\boldsymbol{\omega}_s)\|_{\square}\\ &\le 2\sum_{s=1}^{R}\|\operatorname{diag}(\tilde{\boldsymbol{\omega}}_s-\boldsymbol{\omega}_s)\|_{\square}=2\sum_{s=1}^{R}\|\tilde{\boldsymbol{\omega}}_s-\boldsymbol{\omega}_s\|\le 2\delta\sum_{s=1}^{R}\|\boldsymbol{\omega}_s\|,\end{aligned}$$

where the last line take into account that $\boldsymbol{S}_{\eta_s}$ is the matrix of a downward η_s-position shift for every s. On the other hand, all nonzero entries of $\boldsymbol{S}_{\eta_s}$ are off-diagonal, as long as $\eta_s\neq 0$ for all s, therefore

$$\|\boldsymbol{A}\|\ge\left\|\sum_{s=1}^{R}\mathbb{I}\cdot\operatorname{diag}\boldsymbol{\omega}_s\right\|_{\square}=\left\|\operatorname{diag}\sum_{s=1}^{R}\boldsymbol{\omega}_s\right\|_{\square}=\left\|\sum_{s=1}^{R}\boldsymbol{\omega}_s\right\|\ge\frac{1}{C}\sum_{s=1}^{R}\|\boldsymbol{\omega}_s\|.$$

In the last inequality we use the nonnegativity of $\boldsymbol{\omega}_s$, $1\le s\le R$, as well (31) for the case (b) and the concavity of $t\mapsto\sqrt{t}$ on $(0,\infty)$ for the case (a). □

Constructive proof of Lemma 12

To illustrate how the QTT representation is related to the low-rank decomposition of matrices and can be calculated explicitly, we give also a constructive proof of Lemma 12 below. First, we recapitulate the following notation of [40, 41].

By a *TT core* of rank $r_{k-1}\times r_k$ and mode size $m_k\times n_k$ we denote an array of numbers, which has size $r_{k-1}\times m_k\times n_k\times r_k$. The first and the last indices of a core are called (respectively, *left* and *right*) *rank indices*, while the others are referred to as *mode indices*. Subarrays of a core, corresponding to particular values of rank indices, have size $m_k\times n_k$ and are called *TT blocks*. We may consider the core V_k as an $r_{k-1}\times r_k$-matrix with TT blocks as elements:

$$V_k=\begin{bmatrix}G_{11}&\cdots&G_{1r_k}\\ \vdots&\vdots&\vdots\\ G_{r_{k-1}1}&\cdots&G_{r_{k-1}r_k}\end{bmatrix}=\left[G_{\alpha_{k-1}\alpha_k}\right]_{\substack{\alpha_{k-1}=1,\ldots,r_{k-1}\\ \alpha_k=1,\ldots,r_k}},\tag{52}$$

where $G_{\alpha_{k-1}\alpha_k}$, $\alpha_{k-1}=1,\ldots,r_{k-1}$, $\alpha_k=1,\ldots,r_k$ are TT blocks of V_k, i.e. $V_k(\alpha_{k-1},i_k,j_k,\alpha_k)=\left(G_{\alpha_{k-1}\alpha_k}\right)_{i_kj_k}$ for all values of rank indices α_{k-1},α_k and mode indices i_k,j_k. We refer to this matrix as *core matrix* of V_k.

To avoid confusion, we use parentheses for ordinary matrices, whose entries are numbers and which are multiplied as usual, and square brackets for cores (core matrices), whose entries are blocks and which are multiplied by means of the strong Kronecker product "$\bowtie$" defined below. Addition of cores is meant elementwise.

To ease notation, we omit in TT decompositions like (26), (27) the mode indices with the help of the *strong Kronecker product* [53]. We denote this operation by "$\bowtie$", as in [40, Definition 2.1], where it was introduced as follows, specifically for connecting cores into "tensor trains".

Definition 26 (Strong Kronecker product $\bowtie$ of TT cores)**.** *Consider cores V_1 and V_2 of ranks $r_0 \times r_1$ and $r_1 \times r_2$ and of mode sizes $m_1 \times n_1$ and $m_2 \times n_2$ respectively, composed of blocks $G^{(1)}_{\alpha_0\alpha_1}$ and $G^{(2)}_{\alpha_1\alpha_2}$, $1 \le \alpha_k \le r_k$ for $0 \le k \le 2$. Then the* strong Kronecker product $V_1 \bowtie V_2$ *of V_1 and V_2 is defined as core of rank $r_0 \times r_2$ and mode size $m_1 m_2 \times n_1 n_2$, consisting of blocks*

$$G_{\alpha_0\alpha_2} = \sum_{\alpha_1=1}^{r_1} G^{(1)}_{\alpha_0\alpha_1} \otimes G^{(2)}_{\alpha_1\alpha_2}, \quad 1 \le \alpha_0 \le r_0, \quad 1 \le \alpha_2 \le r_2.$$

In other words, we define $V_1 \bowtie V_2$ as a usual matrix product of the corresponding core matrices, their entries (blocks) being multiplied by means of the Kronecker (tensor) product. For example,

$$\begin{bmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{bmatrix} \bowtie \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix} = \begin{bmatrix} G_{11} \otimes H_{11} + G_{12} \otimes H_{21} & G_{11} \otimes H_{12} + G_{12} \otimes H_{22} \\ G_{21} \otimes H_{11} + G_{22} \otimes H_{21} & G_{21} \otimes H_{12} + G_{22} \otimes H_{22} \end{bmatrix}.$$

Equation (27) can be written then as

$$\boldsymbol{A} = V_1 \bowtie V_2 \bowtie \ldots \bowtie V_{d-1} \bowtie V_d.$$

In the particular case when the second mode length is 1 in each core, the strong Kronecker product of them is a vector and the second mode indices can be omitted. For example, equation (27) reads

$$\boldsymbol{p} = U_1 \bowtie U_2 \bowtie \ldots \bowtie U_{d-1} \bowtie U_d.$$

Constructive proof of Lemma 12 for $J = 2$. For $\lambda \in \mathbb{N}$ and $\mu \in \mathbb{Z} : \ 0 \le \mu < 2^\lambda$ we introduce the vector $\boldsymbol{\sigma}^{(\lambda)}_\mu$ as follows:

$$\boldsymbol{\sigma}^{(\lambda)}_\mu{}_i = \begin{cases} a_1, & 0 \le i < \mu, \\ a_2, & \mu \le i < 2^\lambda, \end{cases}$$

so that $\boldsymbol{\sigma} = \boldsymbol{\sigma}^{(l)}_{\nu_1}$. Let us also denote by $\boldsymbol{e}^{(\lambda)}$ the 2^λ-component vector of ones. For all $\lambda \in \mathbb{N}$ and $\mu = \overline{\mu_\lambda, \ldots, \mu_1}$, where $\mu_k \in \{0, 1\}$ for $1 \le k \le \lambda$, the following recursive relation holds:

$$\boldsymbol{\sigma}^{(\lambda)}_{\overline{\mu_\lambda,\ldots,\mu_1}} = \begin{cases} e_1 \otimes \boldsymbol{\sigma}^{(\lambda-1)}_{\overline{\mu_{\lambda-1},\ldots,\mu_1}} + e_2 \otimes a_2 \boldsymbol{e}^{(\lambda-1)}, & \mu_\lambda = 0, \\ e_1 \otimes a_1 \boldsymbol{e}^{(\lambda-1)} + e_2 \otimes \boldsymbol{\sigma}^{(\lambda-1)}_{\overline{\mu_{\lambda-1},\ldots,\mu_1}}, & \mu_\lambda = 1, \end{cases}$$

where

$$e_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad e_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

which implies a rank-2 representation of the corresponding QTT unfolding matrix and can be recast as

$$\begin{bmatrix} \boldsymbol{\sigma}^{(\lambda)}_{\overline{\mu_\lambda,\ldots,\mu_1}} \\ \boldsymbol{e}^{(\lambda)} \end{bmatrix} = W_2(\mu_\lambda) \bowtie \begin{bmatrix} \boldsymbol{\sigma}^{(\lambda-1)}_{\overline{\mu_{\lambda-1},\ldots,\mu_1}} \\ \boldsymbol{e}^{(\lambda-1)} \end{bmatrix}$$

with

$$W_2(0) = \begin{bmatrix} e_1 & a_2 e_2 \\ & e_1 + e_2 \end{bmatrix} \quad \text{and} \quad W_2(1) = \begin{bmatrix} e_2 & a_1 e_1 \\ & e_1 + e_2 \end{bmatrix}.$$

By unfolding the recursion and selecting the first row corresponding to the vector of interest, we obtain its QTT representation of ranks $2, \ldots, 2$: for $\nu_1 = \overline{\nu_{1,l}, \ldots, \nu_{1,1}}$ we have

$$\boldsymbol{\sigma}_{\nu_1}^{(l)} = U_2(\nu_{1,l}) \bowtie W_2(\nu_{1,l-1}) \bowtie \ldots \bowtie W_2(\nu_{1,2}) \bowtie V_2(\nu_{1,1}) \,,$$

where

$$U_2(0) = \begin{bmatrix} e_1 & a_2 e_2 \end{bmatrix} \quad \text{and} \quad U_2(1) = \begin{bmatrix} e_2 & a_1 e_1 \end{bmatrix},$$

which are the first rows of $W_2(0)$ and $W_2(1)$ respectively, and

$$V_2(0) = \begin{bmatrix} a_2 e_1 + a_2 e_2 \\ e_1 + e_2 \end{bmatrix} \quad \text{and} \quad V_2(1) = \begin{bmatrix} a_1 e_1 + a_2 e_2 \\ e_1 + e_2 \end{bmatrix}.$$

□

For $J > 2$, a similar explicit QTT representation of ranks $J, \ldots, J$ can be obtained by induction in J.

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