MULTIGRID METHODS FOR TENSOR STRUCTURED MARKOV CHAINS WITH LOW RANK APPROXIMATION
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Abstract. Tensor structured Markov chains are part of stochastic models of many practical applications, e.g., in the description of complex production or telephone networks. The most interesting question in Markov chain models is the determination of the stationary distribution as a description of the long term behavior of the system. This involves the computation of the eigenvector corresponding to the dominant eigenvalue or equivalently the solution of a singular linear system of equations. Due to the tensor structure of the models the dimension of the operators grows rapidly and a direct solution without exploiting the tensor structure becomes unfeasible. Algebraic multigrid methods have proven to be efficient when dealing with Markov chains without using tensor structure. In this work we present an approach to adapt the algebraic multigrid framework to the tensor frame, not only using the tensor structure in matrix-vector multiplications, but also tensor structured coarse-grid operators and tensor representations of the solution vector.

Key words. multigrid method, tensor truncation, hierarchical Tucker, Markov chains, singular linear system

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1. Introduction. Consider the stochastic transition matrix $B$ of an irreducible continuous–time Markov chain and the task to find a state vector $x$ such that

$$Bx = 1x,$$

where $x \geq 0$ component wise and the sum of the components is equal to one, i.e., $x$ can be interpreted as a vector of probabilities. Defining $A = I - B$ leads to the problem of solving

$$Ax = 0. \quad (1.1)$$

The matrix $A, A \in \mathbb{R}^{n \times n}$ is singular with corresponding rank $n - 1$ and has column sum zero, i.e., $1^T A = 0$ where $1 = [1, \cdots , 1]^T$. The solution of (1.1) is called the steady state vector and its existence and uniqueness (up to a scalar factor) is proven in [1]. Many continuous–time Markov chains arising in practical applications are known for the so called state space explosion, see, e.g., [13], especially those where the generator matrix $A$ has tensor structure

$$A = \sum_{t=1}^{T} \bigotimes_{j=1}^{J} E_j^t, \quad (1.2)$$

where the matrices $E_j^t \in \mathbb{R}^{n_j \times n_j}$ describe local transitions in each of the $J$ submodels and the other matrices $E_j^t \in \mathbb{R}^{n_j \times n_j}$ the synchronized transitions between the submodels. The sum over the Kronecker products of the matrices gives us the generator matrix of the whole system; cf. [10, 13]. Models of this type appear, e.g., in queueing theory [13, 15, 27] and analysis of stochastic automata networks [34, 39]. Note that most of the $E_j^t, t \neq j$ are the identity matrix and that a rising number of synchronized transitions involves a rising number of summands In addition the dimension

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of $A$ grows exponentially in the number of submodels $J$. Even for moderately large $J$ the storage and computational complexity of forming $A$ explicitly is prohibitive. Thus, in order to be able to do any computations for such models all operations with $A$ have to make use of the compact format (1.2). Due to the fact that $x \in \mathbb{R}^{\prod_{j=1}^{J} n_j}$ it is again difficult to calculate the exact solution due to memory constraints. Thus we assume that the solution $x$ of (1.1) can be approximated by a vector $\tilde{x}$ of the form

$$\tilde{x} = \sum_{i=1}^{R} \bigotimes_{j=1}^{J} x^j_i,$$

(1.3)

with small $R$. This assumption reduces the memory requirements for $x$ from $\prod_{j=1}^{J} n_j$ to $R \sum_{j=1}^{J} n_j$. In addition, using this format matrix-vector multiplications can now be calculated with even smaller computational cost.

The structure of $\tilde{x}$ can be interpreted as an outer vector product, which is equivalent to a $J$-way tensor in the canonical format with tensor rank $R$; cf. [28, 29]. The approximation quality of $\tilde{x}$ depends on its tensor representation; cf. [25]. In this work we focus on the hierarchical Tucker (H-Tucker) format [22, 26, 33] and its performance in a multigrid setting. Recent publications which deal with multigrid methods for Markov chains [2, 7, 12, 17, 18, 19] do not discuss the use of tensors formats in a multigrid context, but show that for simple structured Markov chains a multigrid ansatz often works efficiently. However, recently multigrid has been used [20] to obtain a low rank approximation to speed up the ALS algorithm by exploiting a multilevel structure.

In recent years there have been two main directions in the development of multigrid or multilevel algorithms for Markov chains. On the one hand there are methods based on smoothed aggregation multigrid [17, 18, 19], on the other hand the bootstrap algebraic multigrid framework was also investigated in the context of computing the stationary distribution [2, 7]. In addition in [12] multigrid methods for structured Markov chains like the ones considered in this paper are studied. They are based on aggregation of the submodels and do not maintain the structure of (1.2). Apart from this multigrid approach there are publications which apply to problems with generator matrices of the form (1.2), which have a so called product form solution that can be then computed efficiently [11]. Note that one can interpret our approximation (1.3) of (1.1) as a product form solution if the number of summands is equal to one. Therefore it is obvious to interpret our approach as a combination and generalization of these two established solution techniques. Another recent approach for approximating the stationary distribution of tensor structured Markov chains by a low-rank tensor was presented in [30], based on similar techniques for eigenvalue computations from [31]. This approach does, however, not use multigrid techniques.

The remainder of this work is given as follows. In sections 2 and 3 we give an overview of the basic principles of multigrid methods and tensor formats, respectively. Section 4 gives a detailed explanation on how the individual ingredients of a multigrid method are computed in such a way that the compact format of (1.2) is kept. Section 5 includes a variety of numerical tests and a discussion about the efficiency of our multigrid approach for different choices of building blocks and parameters. Concluding remarks and topics for future research are given in section 6.

2. Multigrid basics. This section gives a brief overview about the concepts of multigrid methods. The building blocks of multigrid methods are smoothing schemes,
the computation of the set of coarse variables, transfer operators and coarse grid operators. In the following there will be only an overview about what these concepts are and how they work together in a multigrid ansatz. For a detailed treatment and motivation we refer the reader to [40]. A prototype of a V-cycle multigrid method is given in Algorithm 1.

### Algorithm 1: Multigrid V-cycle

1. \( v_l = \text{MG}(b_l, v_l) \)
2. if coarsest grid is reached then
3. solve coarse grid equation \( A_l x_l = b_l \).
4. else
5. Perform \( \nu_1 \) smoothing steps for \( A_l x_l = b_l \) with initial guess \( v_l \)
6. Compute the residual \( r_l = b_l - A_l v_l \)
7. Restrict \( b_{l+1} = Q_l r_l \)
8. \( v_{l+1} = 0 \)
9. \( e_{l+1} = \text{MG}(b_{l+1}, v_{l+1}) \)
10. Interpolate \( e_l = P_l e_{l+1} \)
11. \( v_l = v_l + e_l \)
12. Perform \( \nu_2 \) smoothing steps for \( A_l x_l = b_l \) with initial guess \( v_l \)
13. end

The smoothing process typically consists of a few iterations of a simple iterative method like weighted Jacobi, Gauss-Seidel or a Krylov subspace method like Richardson or GMRES; cf. [23, 24, 40]. Afterwards the error \( e \) of the current iterate \( v \) is approximated by approximately solving the residual equation \( A e = r \). This is done by performing the computations on a problem of smaller size on a so called coarse grid. To do so, the residual \( r \) and the operator \( A \) are restricted to a smaller space. In case it is the coarsest level in the hierarchy the restricted system is solved exactly, otherwise the process of smoothing and restriction is repeated until a grid is reached which is small enough for direct computations. Once the coarsest system is solved, the calculated error is interpolated to the next finer grid and added to the current iterate. A final smoothing operation is applied and the process is repeated until the finest grid is reached.

For notational simplicity we use a two grid notation whenever applicable, i.e., all quantities related to the coarse grid have subscript \( c \). In cases where it is necessary to distinguish more than two subsequent grids we use a numbering of the grids as implied by Algorithm 1.

In order to define restriction and interpolation operators one has to specify coarse variables. There are many different approaches available to define them, e.g., geometric coarsening [3], compatible relaxation [4, 6], aggregation [8] and some others which can be found in [40]. Typically these approaches split the variables into two sets, a set of fine variables \( F \) and a set of coarse variables \( C \), which are used in the definition of restriction and interpolation. Assuming that such a splitting is chosen restriction and interpolation operators are described by rectangular matrices. The restriction operator \( Q \) maps the residual to the coarse variables and the interpolation operator from the coarse variables to the original space

\[
Q : \mathbb{R}^{[C \cup F]} \to \mathbb{R}^{|C|} \quad P : \mathbb{R}^{|C|} \to \mathbb{R}^{[C \cup F]}.
\]
There are also many different approaches to build these operators, e.g., least squares interpolation [5, 35], linear interpolation and others [40]. The coarse grid operator $A_c$ is then formed by the Petrov-Galerkin construction $QAP \in \mathbb{R}^{|C|\times|C|}$ and the coarse residual is given by $r_c = Qr$. This is the standard choice in algebraic multigrid methods and gives us the approximated residual equation $A_c e_c = r_c$.

Instead of stopping on the second grid and solving $A_c e_c = r_c$ exactly, e.g., because $A_c$ is still too large, one can again solve this system of equations by a two-grid approach. Iterating this idea ultimately yields a multigrid method, where only on the coarsest grid, i.e., the one with the smallest dimension, the corresponding system is solved exactly. This strategy is described in algorithm 1 and gives rise to a V-cycle depicted in figure 1. Other cycling strategies like W- or F-cycles [40] are also possible, but we do not consider them for the sake of simplicity. However, all ideas developed in this paper can also be used with these cycling strategies in a straightforward way.

3. Tensor basics. In this section we introduce and explain the basic notation and some properties of tensor representations. We define a tensor $\mathcal{X}$ as follows.

**Definition 1.** Consider the space $\mathbb{R} = \mathbb{R}^{n_1} \otimes \cdots \otimes \mathbb{R}^{n_J}$ which is spanned by

$$\{ v^{(1)} \otimes v^{(2)} \otimes \cdots \otimes v^{(J)} : v^{(j)} \in \mathbb{R}^{n_j}, 1 \leq j \leq J \}. \quad (3.1)$$

Then each element $\mathcal{X} \in \mathbb{R}$ is a J-way tensor and the generating products $v^{(1)} \otimes v^{(2)} \otimes \cdots \otimes v^{(J)}$ are called elementary tensors. Note, that one can interpret $\mathcal{X}$ as a multidimensional array.

The rank of a Tensor $\mathcal{X}$ is the smallest integer $r$ that satisfies

$$\mathcal{X} = \sum_{i=1}^r V^{(i)} \quad (3.2)$$

for elementary tensors $V^{(i)}$. 
Note that a one-way tensor is simply a vector and a two-way tensor is a matrix. Any elementary tensor has tensor rank 1. Closely related to tensors is the concept of the Kronecker product.

**Definition 2.** Consider two matrices $A \in \mathbb{R}^{m \times n}$ and $B \in \mathbb{R}^{k \times \ell}$. Then the Kronecker Product of $A$ and $B$ is denoted by

$$A \otimes B = \begin{bmatrix} a_{11}B & a_{12}B & \cdots & a_{1n}B \\ a_{21}B & a_{22}B & \cdots & a_{2n}B \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1}B & a_{m2}B & \cdots & a_{mn}B \end{bmatrix} \in \mathbb{R}^{mk \times n\ell}. \quad (3.3)$$

As the Kronecker product of $J$ vectors $v^{(1)}, v^{(2)}, \ldots, v^{(J)}$, a vector of dimension $n_1n_2\ldots n_J$, and the corresponding tensor $v^{(1)} \otimes v^{(2)} \otimes \cdots \otimes v^{(J)}$ have the same entries we use the same symbol $\otimes$ for tensor and Kronecker products.

We denote the mapping that maps a tensor $X$ to the corresponding vector by $\text{vec}(X)$. The ordering in which the entries appear in the vector is not crucial as long as it is consistent if there are multiple occurrences. A useful property of the Kronecker product is given by the following proposition.

**Proposition 3.** Let the matrices $A, B, C$ and $D$ be given such that the following matrix-matrix products are defined. Then we have

$$(A \otimes B)(C \otimes D) = AC \otimes BD. \quad (3.4)$$

The result of Proposition 3 is of particular interest in the situation that an elementary tensor $X = x^{(1)} \otimes x^{(2)} \otimes \cdots \otimes x^{(J)}$ and a Kronecker product of matrices $A^{(1)} \otimes \cdots \otimes A^{(J)}$ denoted by $\mathcal{A}$ are given such that $A^{(j)}x^{(j)}$ is well-defined. In this situation we find for the multiplication $AX$,

$$\mathcal{A}X = A^{(1)}x^{(1)} \otimes A^{(2)}x^{(2)} \otimes \cdots \otimes A^{(J)}x^{(J)}. \quad (3.5)$$

Thus the product can again be described by an elementary tensor and it can be computed very efficiently by only computing matrix-vector products of small size $n_j$. The following definition gives us the opportunity to generalize this to arbitrary tensors, i.e., tensors with rank larger than one.

**Definition 4.** Consider a tensor $X \in \mathbb{R}^{n_1} \otimes \cdots \otimes \mathbb{R}^{n_J}$. Then the $\mu$-mode product of $X$ with a matrix $U \in \mathbb{R}^{m \times n_\mu}$ is denoted by

$$X \times_\mu U \in \mathbb{R}^{n_1} \otimes \mathbb{R}^{n_{\mu-1}} \otimes \mathbb{R}^{m} \otimes \mathbb{R}^{n_{\mu+1}} \cdots \otimes \mathbb{R}^{n_J}$$

and is given element-wise by

$$(X \times_\mu U)_{i_1i_2\ldots i_{\mu-1}ji_{\mu+1}i_J} = \sum_{k=1}^{n_\mu} x_{i_1i_2\ldots i_{\mu-1}i_jk} \cdot \quad (3.6)$$

We again consider the case that a matrix $\mathcal{A} = A^{(1)} \otimes \cdots \otimes A^{(J)}$ is given and we want to compute $\mathcal{A} \cdot \text{vec}(X)$ for an arbitrary tensor. By using the $\mu$-mode product this amounts to

$$\mathcal{A} \cdot \text{vec}(X) = \text{vec}(X \times_1 A^{(1)} \times_2 A^{(2)} \cdots \times_J A^{(J)}). \quad (3.8)$$
Motivated by the simple matrix-tensor multiplication for elementary tensors it is clear that it is beneficial to work with a tensor representation of $X$ instead of vec $X$, i.e., the full representation. There are many tensor formats (e.g., CP [14, 28, 29], H-Tucker [22, 20], Tensor-Train [36, 37, 38]) with different approximation properties and matrix-tensor multiplications. Of these formats we focus on the CP- and H-Tucker format in the following and introduce their basic concepts next.

3.1. CP-Decomposition. The CP-Decomposition is the simplest compact tensor format. It is based on (3.2) in definition 1. The main advantage of the CP-format is its notational simplicity and storage complexity. To see this, consider the situation that all $n_j$ in (3.1) are equal to $n$, in this case memory storage of an element $X$ is $n^J$ if you use a full representation, i.e., all entries are stored explicitly, and $r \cdot n \cdot J$ if you use (3.2) and just store the vectors defining each elementary tensor. Unless $r \sim n$, this is a substantial saving. Though for the CP representation the rank $r$ has to be known, which is not always the case in practice. Hence in practice you choose a suitable $r$ and approximate $X$ by (3.2) with $r$ terms, denoted by $X_r$. This rank truncation is typically chosen such that $X_r$ is a good approximation to $X$, i.e., the norm of $X - X_r$ is smaller than some prescribed tolerance. The existence of such a low rank approximation $X_r$ is not always guaranteed, see [29]. One way to compute the best rank $r$ approximation is the alternating least squares (ALS) approach, described in algorithm 2.

\begin{algorithm}
\begin{algorithmic}
\State Choose starting values $V^{(1)}, \ldots, V^{(J)}$
\While{not converged}
\For{$j = 1, \ldots, J$}
\State fix all $V^{(k)}, k \neq j$ and solve $\min_{V^{(j)}} \|X - \sum_{i=1}^{r} V^{(i)}\|$ for $V^{(j)}$
\EndFor
\EndWhile
\end{algorithmic}
\end{algorithm}

In here $V^{(i)}$ describes $v_1^{(i)} \otimes v_2^{(i)} \otimes \cdots \otimes v_J^{(i)}$ and $V^{(j)} = [v_1^{(j)} \cdots v_r^{(j)}] \in \mathbb{R}^{n_j \times r}$ collects all vectors corresponding to $j$-th mode of the elementary tensors. In line 4 a least squares problem has to be solved, which can be done by straightforward calculation as it is of small size, see [29]. There are two disadvantages to this approach. First, it is numerically unstable and second, it can only be guaranteed that a local minimum is computed, which may not reach the desired tolerance or requires a non-optimal rank. These disadvantages can be avoided by a hierarchical construction of the tensor approximation as it is done in the Hierarchical Tucker decomposition. We explain its main idea in the next subsection.

3.2. H-Tucker. The H-tucker format is based on the following observation

**Lemma 5 ([22], Lemma 17).** Let $X \in \mathbb{R}^{n_1} \otimes \cdots \otimes \mathbb{R}^{n_J}, t \subseteq \{1, \ldots, J\}$. Consider a partitioning $t = t_1 \cup \ldots \cup t_r, t_i \cap t_j = \emptyset$, then $\text{span}(X^{(t)}) \subseteq \text{span}(X^{(t_r)} \otimes X^{(t)})$, where $X^t$ denotes a matricization of $X$ with respect to the index set $t$, i.e., the matrix in which all modes of $X$ corresponding to the indices in $t$ are merged into rows of $X^{(t)}$ and the modes corresponding to $\{1, \ldots, J\} \setminus t$ are merged into columns, cf. [33].

The consequence of lemma 5 is, that $U^{(t)} = (U^{(t_r)} \otimes U^{(t)}) \cdot B^{(t)}$, where $U^{(t)}, U^{(t_r)}$ and $U^{(t)}$ are bases of the column spaces of $X^{(t)}, X^{(t_r)}$, and $X^{(t_c)}$, respectively, and the matrix $B^{(t)}$ collects the coefficients of the linear combinations describing the
basis $U^{(t)}$ in the basis $U^{(t_{r})} \otimes U^{(t_{ℓ})}$. Therefore, if $U^{(t_{r})}, U^{(t_{ℓ})}$ and $B^{(t)}$ are known, $U^{(t)}$ need not be stored explicitly to have the information about $X^{(t)}$ available. A recursive application of this approach gives us a tree-like structure as illustrated in figure 2. Obviously the dimension tree of a $J$-way tensor contains $J−1$ inner nodes and $J$ leaves (corresponding to single modes). For each leaf a basis $U^{(j)}$ is stored and for each inner node a transfer matrix $B^{(t)}$. Thus the storage complexity is given by $J \cdot n \cdot r + (d − 1) r^3$ if all $n_j$ are equal to $n$ and each basis contains at most $r$ vectors.

For computation of this decomposition there exists a stable algorithm, which is based on singular value decomposition [22, 26].

4. Method. Tensor-based methods are efficient only when the tensors appearing in the problem have low rank. If this is not the case, the tensor structure (1.2) of $A$ can be used to implement fast matrix vector multiplication, but additional savings by using one of the described tensor formats are not possible. Thus the success of our attempt to use a tensor format for the iterates depends crucially on the rank of the steady state vector. The following two theoretical results shed some light on this matter.

**Theorem 6 ([11, Theorem 2]).** For a non-interacting system, i.e., $E_{ij} = I$ for $i \neq j$ and $T = J$ in (1.2) the stationary distribution $p$ satisfies

$$ p = \bigotimes_{j=1}^{J} p^{(j)}, \quad (4.1) $$

where $p^{(j)}$ is the stationary distribution of $E^{(j)}_{ij}$, i.e., it corresponds to a tensor of rank one.

The proof is simple, as obviously the tensor product of the individual stationary distributions of the systems is the stationary distribution of the combined system. For less trivial systems a similar but much weaker result can be stated, given by the following theorem.

**Theorem 7 ([11, Theorem 1]).** For every matrix of the form (1.2) the stationary distribution is representable as a tensor of rank at most $n/(\max_j n_j)$, where $n = \prod_{j=1}^{J} n_j$.

Therefore, the introduction of truncation and the use of efficient tensor formats and thus saving of memory and compute time should be possible, assuming that
the stationary distribution is a $J$-way Tensor with bounded rank. Of course, these
theorems only cover the extremal cases which can occur. A representation with the
maximal possible rank given by Theorem 7 would not be efficient in practice (as this
bound grows exponentially in $J$), so that this result is more of theoretical interest. On
the other hand, Theorem 6 suggests that for systems with a low level of interaction an
approximation of the stationary distribution by a tensor with very low rank should be
possible. Although no better upper bounds than the one from Theorem 7 are known,
umerical experiments in, e.g., [30] as well as our experiments in section 5 show that
in practice a rather low rank is often sufficient.

These results motivate the development of multigrid methods for system matrices $A$
with tensor structure that allow for the efficient use of tensor formats like the ones
described in section 3. In the following we will describe the chosen building blocks of
the multigrid method that need to be specified as discussed in section 2. Our main
goal in the following is to preserve the tensor structure of $A$ in (1.2).

We begin with the choice of the transfer operators $P$ and $Q$. The following
proposition gives us a starting point for achieving our goal of maintaining the structure
of $A$.

**Proposition 8.** Let $A$ of the form (1.2) be given with $E_{j}^{t} \in \mathbb{R}^{{n_{j}^t} \times {n_{j}^t}}$. Let $P = \bigotimes_{j=1}^{J} P_j$ and $Q = \bigotimes_{j=1}^{J} Q_j$ with $P_j \in \mathbb{R}^{{n_{j}^c} \times {n_{j}^c}}$ and $Q_j \in \mathbb{R}^{{n_{j}^c} \times {n_{j}^c}}$ where $n_{j}^c << n_{j}$.

Then the corresponding Petrov-Galerkin operator satisfies

$$QAP = \sum_{t=1}^{T} \bigotimes_{j=1}^{J} Q_j E_{j}^{t} P_j.$$  

(4.2)

**Proof.** By using Proposition 3 repeatedly, we have for each $t$

$$\left( \bigotimes_{j=1}^{J} Q_j \right) \left( \bigotimes_{j=1}^{J} E_{j}^{t} \right) \left( \bigotimes_{j=1}^{J} P_j \right) = \left( \bigotimes_{j=1}^{J} Q_j E_{j}^{t} \right) \left( \bigotimes_{j=1}^{J} P_j \right) = \bigotimes_{j=1}^{J} Q_j E_{j}^{t} P_j.$$  

(4.3)

The assertion follows by linearity of the Kronecker product.  

This way of forming $P$ and $Q$ directly implies that they are built with respect to the “local” operators $E_{j}^{t}$ of smaller dimension and lifted to the full dimension of $A$
via Kronecker products. The exact choice of the small interpolation and restriction
operators $P_j$ and $Q_j$ depends on the considered problem. In principle all known
constructions from algebraic multigrid can be used. In section 5 we give details on
how the transfer operators are computed for each of the considered examples.

Another direct consequence of proposition 8 is that the set of coarse variables can
be computed for the smaller problems described by the matrices $E_{j}^{t}$. However, it is
not always straightforward how to do this. In case the matrices $E_{j}^{t}$ originate from
some nice geometric structure, like the overflow queuing network example in section
5.1, you can use an established coarsening algorithm. A matrix like in the Kanban
system example in section 5.2 does not correspond to a connected graph, indeed there
are several isolated states. In this case, coarsening can, e.g., be done with respect to
the auxiliary matrices

$$\bar{E}_{j} = \sum_{t=1}^{T} E_{j}^{t},$$  

(4.4)

which collect all transitions of the $j$-th subsystem and therefore corresponds to a
connected graph again. Problems of the first kind can be thought of $j$ individual
Markov chains which are coupled in some way, but are also meaningful on their own, while the second kind are systems which have a very high level of interaction where each individual subsystem is dysfunctional without interaction with the other systems. This will be seen in more detail in the description of the different test examples in section 5.

In summary, by keeping in mind these considerations, we are able to maintain the tensor structure of the system matrix $A$ throughout all levels of our multigrid method. This structure has two main advantages: First, only the small matrices need to be stored, substantially reducing the storage requirements and second, by using (3.8) an efficient matrix vector product can be performed if $X$ is given in one of the tensor formats described in section 3 with low rank. Here and throughout the rest of the paper by rank we mean the tensor rank in the sense of definition 1 in case of the CP format and the maximum number of basis vectors across all nodes of the dimension tree in case of H-Tucker.

We first illustrate the efficient matrix vector product and its implications for the CP format, as this format allows for the least notational overhead, and then state the precise results also for the other formats. Consider a tensor $x \in \mathbb{R}^n$ with the same tensor structure as the matrix $A$ in (1.2), i.e.,

$$
x = \sum_{i=1}^{r} \otimes_{j=1}^{J} v_{j}^r,
$$

then the matrix vector product is given by

$$
Ax = \sum_{t=1}^{T} \sum_{i=1}^{r} \otimes_{j=1}^{J} E_{t}^j v_{j}^r.
$$

(4.5)

It is obvious that substantial saving in computational and storage complexity is realized if $r$ is small enough, but for $Ax$ we already need the same storage as for a $r \cdot T$-rank tensor. Thus with every multiplication with $A$ the rank of our tensor increases by a factor of up to $T$, to avoid this, $Ax$ should be approximated by $r$ summands again. This technique is known as truncation and is widely used in algorithms for tensor structured problems, see, e.g., [22, 26, 31, 32]. In case of the CP-format you can use the ALS algorithm for truncation. In our method we truncate our iterate after every multiplication with $A$. This only makes sense if the complexity is smaller than for the explicit matrix vector multiplication in the sense of storage and computational cost which is typically the case when $T$ and/or the matrix dimension of $A$ is large.

Remark 1. The above presentation also applies in almost the same way for the H-Tucker tensor format, which can be seen as follows. By using (3.8) we can multiply $A$ with an arbitrary tensor in an efficient way as long as the $\mu$-mode product and addition of tensors can be performed at low cost in the chosen format. For H-Tucker, the $\mu$-mode product with a matrix $A^{(\mu)}$ just means replacing the basis matrix $U_{\mu}$ by $A^{(\mu)} U_{\mu}$. The rank increase due to addition of tensors observed for the CP format is also present in the H-Tucker format. Addition of two tensors is performed by concatenating the basis matrices of both tensors and embedding the transfer tensors into block diagonal tensors, see [33]. Truncation can, just as for CP, be achieved by the algorithms used to convert tensors into the H-Tucker format. Note, however, that there exist more efficient truncation algorithms for this format if $X$ already is in H-Tucker format but with a too large rank [22].
The coarse grid operator is chosen as the Petrov-Galerkin operator, i.e., $A_c = QAP$, being the natural extension of the Galerkin operator that is the optimal coarse grid operator in the symmetric case.

After interpolation and restriction have been chosen and the coarse matrix has been defined, an appropriate smoother has to be chosen. To benefit from the possible savings that an efficient matrix vector multiplication as discussed before provides, the smoother has to use matrix vector products rather than point-wise operations, thus methods like SOR or Kaczmarz are no viable options. With this limitation the obvious choice are Krylov subspace methods like GMRES, as they only require matrix vector products, or Richardson, which only needs scaled vector updates. Another choice is Jacobi, as it does not require a traditional point-wise update of the vector components but rather a scaling using a diagonal matrix. The diagonal matrix can be represented using a vector and this vector can be inverted element-wise. Using a truncated tensor representation of this vector and approximating the element-wise inversion using a Newton-Schultz iteration as implemented in the h Tucker-Toolbox\textsuperscript{[33]} hence the smoother can be implemented efficiently exploiting the tensor structure.

Finally, on the coarsest grid the residual equation has to be solved. There are two ways to do this, either the coarsening results in a problem of a size where direct solving without exploiting tensor structure is possible or an iterative method (e.g., GMRES) is used. In both cases truncation has to be applied to obtain a low rank tensor representation of the solution.

5. Numerical Tests. In this section we illustrate how to choose the ingredients of a multigrid approach based on two examples. All computations were performed in MATLAB R2013a using the h Tucker-Toolbox\textsuperscript{[33]}.

5.1. Overflow queuing network. The first example we consider is the so called Overflow Queuing Network. A finite number $J$ of queues is given with a corresponding capacity $k_i$, $i = 1, \ldots, J$. Customers arrive to an arbitrary queue $q_i$, $i = 1, \ldots, J$ according to a Poisson process with rate $\lambda_i$, $i = 1, \ldots, J$ and are served with an exponentially distributed service time with rate $\mu_i$, $i = 1, \ldots, J$. These local processes can be described by the following matrices

$$E_i^{(i,i)} = \begin{pmatrix} 0 & \mu_i & & \\
0 & \lambda_i & \ddots & \\
& \ddots & \ddots & \ddots \\
& & \ddots & \mu_i \\
0 & & & \lambda_i & 0 \end{pmatrix}, \quad i = 1, \ldots, J. \quad (5.1)$$

Note that here and in the following, for a better understanding we denote the transitions by two-tuples instead of natural numbers. Here, the tuple $(i, j)$ describes a transition which is initiated by queue $i$ and affects queue $j$. The synchronized events appear if queue $q_i$ has reached its capacity, i.e., $q_i$ is full. In this situation an arriving customer has to enter $q_{i+1}$. If $q_{i+1}$ is also full, the customer will enter the subsequent queue $q_{i+2}$ and so on. If all of the subsequent queues are full, the customer will leave the system. For sake of simplicity we only describe the synchronized events in which the customer can enter the subsequent queue, because it is not full.
• if $q_i$ is full, the customer leaves $q_i$, which leads to the following matrix

$$E^{(i,i+1)}_i = \begin{pmatrix} 0 & 0 \\ 0 & \ddots \\ \vdots & \ddots & 0 \\ 0 & \ddots & 0 & 0 \\ 0 & \lambda_i \end{pmatrix}, \ i = 1, \ldots, J - 1.$$

• if $q_i$ is full, $q_{i+1}$ gets an additional customer, which leads to the following matrix

$$E^{(i,i-1)}_i = \begin{pmatrix} 0 & 0 & 0 \\ 1 & \ddots & \ddots \\ \vdots & \ddots & 0 \\ 0 & \ddots & 0 & 1 & 0 \\ 0 & \ddots & \ddots & \ddots & 1 \end{pmatrix}, \ i = 2, \ldots, J.$$

For a detailed description of the model see [10]. Note that the choices of the parameters $\lambda$ and $\mu$ affect whether more synchronized or local events appear. For a better understanding, consider 3 queues with capacity 17 and different choices of the parameters $\mu = [\mu_1, \ldots, \mu_J]$ and $\lambda = [\lambda_1, \ldots, \lambda_J]$, which can be seen in figure 3. The figures 3a, 3b, and 3c show the distributions of the solutions for the corresponding parameter choice on each queue. In every figure we have three axes (one for each queue) and each axis describes the capacity. In case customers arrive slowly and are served rapidly (small $\lambda$, large $\mu$) all queues are (almost) empty; cf. figure 3a. On the other hand, if customers arrive in short succession and are served slowly we obtain a steady state solution that corresponds to three full queues as can be seen in figure 3b. Both parameter sets have limited interaction, in the first situation no queue ever flows over which results in no interaction and in the second case almost every customer that is rejected at a queue is rejected at each subsequent queue as well, resulting effectively in no interaction as well. Only if the parameters are chosen such that slow and fast queues are mixed the steady state distribution becomes non-trivial as can be seen in 3c. In figure 4 we investigate the best rank approximation for the three different problems and observe that for the solution 3c a higher rank is needed than for the other ones. This observation confirms the assumption that a higher level of interaction in the model leads to a higher rank for its solution. Nevertheless, an accurate approximation of the solution is still obtainable with low rank.

One way to choose the ingredients for a multigrid approach is to take into account the underlying geometric structure and to preserve some important properties of the problem matrix $A$ on the coarse grids. In our case, the property that our matrix $A$ has column sum zero should be kept. The structure of our overflow queuing problem for $J = 3$, $k = [8, 8, 8]$ is shown in Figure 5. Note that the nonzero structure is exactly the same as that of the standard finite difference discretization of the $J$-dimensional Laplace operator. A look at the geometric structure of the local problem in an overflow queuing problem (5.1) and the structural similarity to the Laplace operator motivated us to use full coarsening and direct interpolation for the interpolation operator, based on these local matrices, for each queue. To keep the column sum of the coarse grid
Fig. 3: Solution for parameters (a) $\mu = [1, 1, 1]$ and $\lambda = [0.1, 0.1, 0.1]$, (b) $\mu = [0.1, 0.1, 0.1]$ and $\lambda = [1, 1, 1]$, (c) $\mu = [0.25, 0.5, 1]$ and $\lambda = [0.5, 0.5, 0.5]$.

Fig. 4: Best rank $R$ approximations for parameters (a) $\mu = [1, 1, 1]$ and $\lambda = [0.1, 0.1, 0.1]$, (b) $\mu = [0.1, 0.1, 0.1]$ and $\lambda = [1, 1, 1]$, (c) $\mu = [0.25, 0.5, 1]$ and $\lambda = [0.5, 0.5, 0.5]$.

matrix zero, we use linear restriction, because our coarse grid matrix is a Petrov–Galerkin operator and we then have $1^T Q A P = 1^T A P = 0$ as the linear restriction operator $Q$ fulfills $1^T Q = 1$.

For the first numerical test, we choose $J = 5$, $\lambda = [1.2, 1.1, 1.0, 0.9, 0.8]$, $\mu = [1, 1, 1, 1, 1]$ and $\kappa = [16, 16, 16, 16, 16]$. This leads to a problem size of $17^5 = 1,419,857$. We apply our multigrid method with 4 levels, and use an implementation of GMRES that exploits the tensor structure in matrix vector products and inner products as the smoother and perform 3 pre- and postsmoothing steps. We use the Moore–Penrose pseudoinverse to solve the singular coarse grid system. As initial guess we use the smallest singular vector from the matrix corresponding to the smallest grid and interpolate it up to the original dimension, which can be done in the setup at low cost. In experiments we could observe that this typically leads to a better starting point than a random initial guess. The availability of this starting guess is an additional advantage of a multigrid approach in this context. Note that after every V-cycle we normalize our iterate to guarantee that $1^T x = 1$.

In our first experiments we fix the truncation rank. Figure [6a] shows these experiments for a truncation rank ranging from 20 to 320. Note that the accuracy is given by the relative norm $\frac{\|Ax\|}{\|x\|}$. We observe that for this kind of problem a higher
Fig. 5: Nonzero structure of overflow queuing network for $J = 3, k = [8, 8, 8]$.

Fig. 6: Convergence history for $J = 5, k = [16, 16, 16, 16, 16]$ with (a) different fixed truncation ranks and (b) adaptive rank increase.

A truncation rank is needed for a better accuracy. But a higher truncation rank means more computational cost. Here we have another advantage of our multigrid approach, namely that we are able to increase the rank adaptively, i.e., after every V-cycle we check whether we have a certain percentage of increase of the accuracy. If this is not the case we increase the rank, in our implementation we double the current truncation rank. Figure [b] shows the convergence process with the integrated adaptive rank increase. Here the connection between Figure [a] and [b] is distinctive. The occurring stagnations in figure [a] imply a rank increase in our method, which then leads to a faster convergence until stagnation occurs again and the rank has to be increased further. Of course, the overall convergence will be faster (in number of iterations)
Tables 1 and 2 show the number of iterations and truncation rank needed for different test problems. For these problems we use three stopping criteria:

- accuracy of at least $10^{-8}$,
- maximum number of 30 iterations,
- maximum truncation rank of 320.

The effective stopping criterion is included in the tables. Note that we fix the number of three pre- and postsmoothing steps and that in each model every queue has the same capacity $k_i = kk, i = 1, \ldots, J$.

The numerical tests show that for problems with $J = 4$ the iteration number scales very nicely with the problem size. A comparison of $kk = 8$ and $kk = 32$ shows that the iteration count increases by about fifty percent while the dimension of the problem increases by a factor about 180. Unfortunately, both an increase of $kk$ or $J$ leads to a higher rank of the solution, therefore causing problems if both values are increased (e.g., line 5 and 6 in table 1).

### 5.2. Manufacturing system with Kanban control.

The second example we consider is the so called Kanban model as it is discussed in [9]. A finite number $J$ of cells is given and each of them contains a machine, a bulletin board and an output hopper. Parts have to go through these machines in a certain order. We assume that this order is given by the numeration of the machines. Only a certain number $k_i, i, \ldots, J$ of parts can enter a machine, which is controlled by the so called Kanban tickets, i.e., $k_i$ is the number of existing Kanban tickets for machine $i$. Each part which enters a machine gets a Kanban ticket and gives it back when it enters the subsequent machine. If no tickets are available in machine $i$ the part has to wait in the output hopper.
hopper of the previous cell $i - 1$ before entering the machine. The processing time
and the time to move from one cell to the next are exponentially distributed with rate
$\mu_i$ and rate $\omega_i$, respectively. As in the previous example we want to distinguish the
local events and the synchronized ones. Note that the synchronized events exist only
between neighboring machines. For sake of simplicity we initially do not consider the
first and the last machine. Each machine can be described by a Markov chain, where
each state is characterized by three quantities:

- number of available tickets,
- number of parts being processed,
- number of parts waiting for the next machine.

In Figure 7 we illustrate the states of one machine with five tickets and characteri-
tize their transitions from one state to another as local or synchronized, where local
transitions are the ones that are independent of the neighboring machines, i.e., the
transition from the machine to the output hopper.

Ordering the states lexicographically and distinguishing the three different types
of transitions, we find three different graphs corresponding to one machine, as depicted
in Figure 8. The matrices describing the different transition types are exactly the
transpose of the adjacency matrices of these graphs, with all nonzero entries equal to
$\mu_i$ (for local transitions), $\omega_{i-1}$ (for transitions depending on the previous machine).
or $\omega_i$ (for transitions depending on the subsequent machine). In the local transition matrix, additionally the diagonal entries of nonzero columns are set to be $-\mu_i$. The corresponding matrices for a machine with two tickets are given as follows:

$$E^{(i,i)}_1 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\mu_i & 0 & 0 & 0 & 0 \\ 0 & \mu_i & 0 & 0 & 0 & 0 \\ 0 & 0 & -\mu_i & 0 & 0 & 0 \\ 0 & 0 & 0 & \mu_i & -\mu_i & 0 \\ 0 & 0 & 0 & 0 & \mu_i & 0 \end{pmatrix}, \quad E^{(i,i-1)}_2 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ \omega_{i-1} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \omega_{i-1} & 0 & 0 & 0 \\ 0 & 0 & 0 & \omega_{i-1} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$E^{(i,i+1)}_i = \begin{pmatrix} 0 & 0 & \omega_i & 0 & 0 & 0 \\ 0 & 0 & 0 & \omega_i & 0 & 0 \\ 0 & 0 & 0 & 0 & \omega_i & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad i = 2, \ldots, J - 1. \tag{5.2}$$

The difference of the first and the last machine to the others is that they have only one neighbor, so the number of states of the corresponding Markov chain is smaller. To be more precise, the last machine lacks an output hopper (i.e., as soon as a part is finished its ticket is available), whereas the first machine has no bulletin boards (i.e., in case there are tickets available, a new part immediately enters the machine). Thus both the first and the last machine can be described by only two of the three state quantities. As such the states for the first and the last machine can also be read from figure 7. The first row of the state triangle describes the last machine and the first machine is given by the right-most diagonal.

The sparsity structure of the whole system with three machines and five tickets each is given in figure 8. In contrast to the overflow queuing model the graphs corresponding to the local matrices have some unreachable states, thus full coarsening with these matrices is not possible and in addition the geometric structure of these matrices does not bear a likeness to the structure of the system matrix depicted in
figure 9 for example they have some zero columns. We thus base our coarsening approach on the accumulated local structure as shown in figure 7 and use a simple aggregation approach with constant basis function. On the left of figure 10 the selected aggregates for a problem with five tickets are shown. For the first and last machine the aggregates are chosen accordingly based on the identification with the right-most diagonal and first row, respectively. By enumerating the aggregates along the diagonals of the grid (starting in the upper left corner, just like the original numbering of the nodes in Figure 8) we preserve the connection structure of figure 7 and thus are able to continue aggregating according to this geometry to end up with a multilevel approach. On the right of figure 10 the choice of aggregates for further coarsening to a third level are shown. Note that the number of tickets in one machine should be $2^k + 1$ to allow for such an aggregation and we limit our analysis to such Kanban systems. This limitation is simply a technical issue and we suspect that irregular numbers of tickets can be dealt with by adapting the aggregation accordingly.

For our numerical tests we choose the aggregation approach as described before, therefore the choice of interpolation and restriction operator is given by standard aggregation interpolation (the restriction operator is just the transpose of the interpolation operator), see, e.g., [41], and the coarse grid matrix $A_c$ is the corresponding (Petrov–)Galerkin operator as before. Note that the column sum of $A_c$ is equal zero, because every column in the restriction matrix has only one entry with the value one. As a smoother, we use ten steps of a weighted Jacobi iteration, see, e.g., [23, 40] on the finest grid and three steps of GMRES on coarser grids. Some numerical tests

![Diagram](image-url)
showed that GMRES does not work well as a smoother for Kanban problems in contrast to weighted Jacobi on the finest level. As it turned out to be troublesome and expensive for the aforementioned Newton-Schulz method to converge to a satisfactory accuracy on coarser levels, we use Jacobi only on the finest grid. Fortunately, the difference between GMRES and Jacobi is not as significant on the coarser grids, so that a satisfactory convergence behavior can be observed.

The other ingredients of the method are the same as in example \(5.1\). The stopping criteria are:

- accuracy of at least \(10^{-8}\),
- maximum number of 30 iterations,
- maximum truncation rank of 160.

Table 3 and 4 show the results of some numerical tests for different numbers of machines and tickets. We can observe that the method works well for all tested problems, in some cases it seems that it would be better to start with a higher rank in order to reach a better accuracy. Again we see that a higher rank is needed with increasing dimensions of the problem. Apart from the rank increase we can again observe that the method scales reasonably well with growing problem size.

6. Conclusion. We discussed how to develop multigrid methods for tensor-structured problems, specifically structured Markov chains, which on the one hand exploit the tensor structure for efficient matrix and vector operations and at the same time keep this structure intact across all grids. We illustrated the behavior of our method by investigating two standard model problems.

Topics for future research include investigating the use of different tensor formats, e.g., Tensor Train, in the context of multigrid approaches and exploring different coarsening strategies, e.g., aggregation across submodels (i.e., queues or machines for the overflow queuing or Kanban system, respectively) for very large scale problems.

A further extension of this work is generalizing the structure-preserving multigrid approach to other classes of structured Markov chains, e.g., multi-server multi-queue models.

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