Abstract Since its introduction by Gauss, *Matrix Algebra* has facilitated understanding of scientific problems, hiding distracting details and finding more elegant and efficient ways of computational solving. Today's largest problems, which often originate from multidimensional data, might profit from even higher levels of abstraction. We developed a framework for *solving tensor structured problems with tensor algebra* that unifies concepts from tensor analysis, multilinear algebra and multidimensional signal processing. In contrast to the conventional matrix approach, it allows the formulation of multidimensional problems, in a multidimensional way, preserving structure and data coherence; and the implementation of automated optimizations of solving algorithms, based on the commutativity of all tensor operations. Its ability to handle large scientific tasks is showcased by a real-world, 4D medical imaging problem, with more than 30 million unknown parameters solved on a current, inexpensive hardware. This significantly surpassed the best published matrix-based approach.

Keywords Tensor · Multidimensional problems · Tensor computations · Tensor equations · Tensor solvers

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1 Introduction

Computational problems with tensor structure, which involve large amounts of multidimensional data, arise in many fields of science and engineering.
The standard way of dealing with such problems is not intrinsically multidimensional, and assumes reduction of problem formulation to the classical matrix formalism, which is built on two-dimensional (matrix) and one-dimensional (vector) data structures. This is achieved by the reordering of multidimensional terms from the original problem formulation, into matrices and vectors. The derived matrix formulation is then treated using well-known techniques and algorithms of matrix algebra. Finally the solution is reconstituted into its natural multidimensional form.

While this approach reduces a multidimensional problem to the well-known standard form of matrix algebra, it introduces certain limitations. The resulting formulation is no longer explicitly multidimensional, - a fact that may create difficulty in identifying and understanding important properties inherent to the particular problem [20]. Vectorization of multidimensional objects may lead to loss of spatial data coherence [6,13], which can adversely affect the performance of solving algorithms. In many cases, the derived problem formulation does not have a straightforward, intuitive connection with the process of generating efficient solving algorithms.

Currently, a growing interest in objects with more then two dimensions – tensors, has become evident in the scientific community. Introduced in Tensor Analysis and Multilinear Algebra, tensors gained the attention of practitioners of diverse fields (see the excellent review by Kolda [14]). However, translating tensor mathematics to a convenient computational framework raises many issues [19]; including, convenient notation, ease of algorithm implementation, performance.

Here we propose a comprehensive framework for solving tensor structured problems by tensor algebra that allows natural and elegant formulation of multidimensional problems using multidimensional data structure directly. The proposed framework is based on a generalization of the concepts of matrix algebra to multiple dimensions; it incorporates and unifies existing approaches from multidimensional signal processing [5,10,3], recent developments in the field of tensor analysis [12], and multilinear algebra [27,17,16,11,14,19]. It is based on ordered vector spaces and a generalized definition of tensor multiplication, based on the concept of tensor equations and the tensor inverse, and induces the design of fast computational solving algorithms with built-in expression analysis for automated generation of efficient implementations on serial and parallel computers. In our companion paper we show how to computationally solve large real-world problems using our framework, and claim that this novel approach offers a natural, higher level abstraction to solving a broad range of very large computational problems which arise in multidimensional signal processing and other scientific fields.

2 Tensor nomenclature, basic tensor operations

In our framework, multidimensional data and multidimensional transformations are described based on a formalism originating in Tensor Analysis [12]
Each object in the formulation represents a multidimensional entity – a tensor. Tensors describing multidimensional data belong to a space that is the outer product of a number of vector spaces (see A.3). A tensor can be represented by a multidimensional array of its components. For example, a scalar field defined on a discrete uniform three-dimensional grid with extents \([N_X, N_Y, N_Z]\) can be expressed as a third order tensor \(\mathcal{T}^{xyz}\), where tensor order is determined by the number of indices. Note that in our tensor notation, direct correspondence between designation of tensor indices \((x, y, z)\) and dimensions of the physical space \((X, Y, Z)\) is typically used. Tensors indices can be either covariant (subscripts) or contravariant (superscripts), depending on the way the tensor components transform in respect to a change of basis (see A.1). This property of a tensor index is called variance. For the common case of Euclidean spaces with orthonormal bases, there is no difference between covariant and contravariant indices; thus the choice of index variance is influenced by the context and consistency of tensor expressions.

Consider a transformation applied to tensor \(\mathcal{T}^{xyz}\) which results in a tensor in the same tensor product space. The transformation can be expressed by \(A_{xyz}^{x'y'z'}\). Its application to \(\mathcal{T}\) implies the use of classical tensor operations, such as the outer product, which expands tensor order

\[
A_{xyz}^{x'y'z'} \cdot \mathcal{T}^{xyz} = C_{x'y'z'}^{xyz}
\]

and the contraction, which reduces tensor order

\[
C_{x'y'z'}^{xyz} \equiv \sum_x \sum_y \sum_z C_{x'y'z'}^{xyz} = D^{x'y'z'}
\]

For designation of the contraction, we use the Einstein convention [7] which assumes implicit summation over a pair of indices with equal designation but different variance. From the practical point of view, it is convenient to combine the outer product and the contraction into a single operation, in analogy with the matrix multiplication. Thus by allowing simultaneous contraction over multiple corresponding index pairs we get

\[
A_{xyz}^{x'y'z'} \cdot \mathcal{T}^{xyz} = D^{x'y'z'}
\]

Our framework relies on the fact that a tensor is an object which can implicitly contain all its properties as indices and component values. Due to this object nature in a practical implementation (2.3) can be reduced to \(D := A^*T\), where "*" denotes tensor multiplication.

2.1 Concept of ordered spaces, commutativity of tensor multiplication

In some cases, multidimensional transformations can be decomposed to a product of one-dimensional transformations. Such transformations are called sepa-

\[1\] Further in the document the term tensor is identified with tensor components
vable. They are reduced to sequential application of one-dimensional transformations from the decomposition. Using tensor formalism in three dimensions this can be expressed as

$$A_{x'y'z'}^x \cdot T_{xyz}^x = B_{y'}^y \cdot C_{z'}^z \cdot D_{z}^z \cdot T_{xyz}^y = E_{z'y'z'}^z \quad (2.4)$$

In conventional tensor formalism (and likewise in matrix formalism), the result of expression (2.4) depends on the order of multiplicands (lack of commutativity). This is due to concatenation of non contracted indices, which is used for assurance of a unique result of the tensor product. In contrast, separable data handling operations, like filtering or resampling in signal processing, lead to the same result independently of the order in which separable transformations are applied. To avoid this formal, but practically important mismatch, and to add more flexibility to handling of tensor expressions, we introduce the following constraint: in analogy to physical space, which is ordered (right hand rule), we require vector spaces used for construction of the tensor product to have a unique predefined order. This constraint leads to a fundamental new property of the framework, compared to conventional approaches for matrix and tensors. The tensor multiplication becomes commutative, in addition to being associative. Formally this means that indices of the resulted tensor have unique positions determined by a predefined order of vector spaces. Thus complex tensor products can be evaluated in arbitrary order but lead to the same result. For example, for ordered spaces $X, Y, Z$ we can write

$$A_{x'y'z'}^x \cdot B_{y'}^y \cdot C_{z'}^z \cdot T_{xyz}^y = B_{y'}^y \cdot A_{x'y'z'}^x \cdot C_{z'}^z \cdot T_{xyz}^z = B_{y'}^y \cdot C_{z'}^z \cdot A_{x'y'z'}^x \cdot T_{xyz}^z = E_{z'y'z'}^z \quad (2.5)$$

The commutativity of the tensor multiplication, achieved hereby, considerably increases the ease of handling tensor expressions. One of the important practical values of this property consists in simplification of semantic analysis of tensor expressions performed for the purpose of reduction of computational and storage requirements. For example, expression $A_{x't}^x \cdot B_{y'}^y \cdot C_{z'}^z \cdot T_{xyz}^y$, $(N_X < N_Y < N_Z < N_T, N_X N_Y > N_T)$, which according to conventional tensor and matrix formalisms can be evaluated only in a single chain order, in our framework can be computed by reordering $C^z_{z'} \cdot (B_{y'}^y \cdot (A_{x't}^x \cdot T_{xyz}^y))$. This gives the best computational performance with minimal memory requirements for storing intermediate results. At this point, it is possible to use the tensor multiplication, in combination with tensor addition and subtraction, defined from multilinearity of tensor product space (see [A.23] for formulating multidimensional problems in a natural and elegant multidimensional representation. Note

\[ ^2 \text{ With operations on mixed tensors, it can be rather difficult to track the overall order of array indices in the results. Thus in some tensor literature a special notation is used, where unique index order is defined by use of "dot" symbol (E_{x'y'z'}). But this brings an undesirable side-effect in significantly decreasing the readability of tensor expressions.} \]

\[ ^3 \text{ Note that this constraint does not limit the expressiveness of tensors, as the order of vector spaces can be changed if necessary.} \]
that formulations expressed in tensor terms are also convenient for differentiation in respect to multidimensional terms (see A.8), an important prerequisite for multidimensional optimization problems.

2.2 Extension of the tensor notation

According to Einstein notation it is not permitted to have more than one index with same designation and variance. However, in our settings we do allow this, with agreement on some consistency rules. As an example, consider the following expression

\[ A^i_i \cdot B^i_y = H^i_{xy} \]  \hspace{1cm} (2.6)

This operation is a tensor analogue of the Khatri-Rao product [26] which is a matching elementwise (over \( i \)) Kronecker product of two sets of vectors. Note that two formally equivalent indices are merged into a single one, without dependency on outer product or contraction applied to other indices. But the constraint is, that indices can be contracted only once after all possible merges resulting in a single pair of superscript and subscript. Here is an example which represents the most general form of the tensor product, combining outer product, contraction and elementwise product

\[ A^i_x \cdot D^z_i \cdot B^i_y \cdot P_{iz} \cdot W_i = (A^i_x \cdot B^i_y) \cdot (D^z_i \cdot P_{iz} \cdot W_i) = H^i_{xy} \cdot N^z_{iz} = R_{yz} \]  \hspace{1cm} (2.7)

Notice how neatly the proposed notation unifies different types of products which exist separately in Matrix Algebra (Matrix product, Kronecker product, Khatri-Rao product).

3 Tensor equations and tensor inverse

Expression \( A^{x_1 y_1 z_1}_{x_2 y_2 z_2} \cdot U^{x_2 y_2 z_2} = B^{x_1 y_1 z_1} \) represents a relation between a multidimensional input \( U^{x_2 y_2 z_2} \) and a multidimensional output \( B^{x_1 y_1 z_1} \). This relation is determined by a transformation \( A^{x_1 y_1 z_1}_{x_2 y_2 z_2} \). When the input is unknown, the expression describes an inverse problem. In cases where a unique solution exists, the existence of a tensor inverse is implied – a transformation which maps \( A \) to the identity tensor

\[ \delta^{x_2 y_2 z_2}_{x_1 y_1 z_1} \cdot A^{x_1 y_1 z_1}_{x_2 y_2 z_2} \cdot U^{x_2 y_2 z_2} = \delta^{x_2 y_2 z_2}_{x_1 y_1 z_1} \cdot U^{x_2 y_2 z_2} = U^{x_2 y_2 z_2} \]  \hspace{1cm} (3.1)

where \( \delta^{x_2 y_2 z_2}_{x_1 y_1 z_1} \) is the identity transformation in three dimensions expressed in terms of Kronecker delta (see A.5). Note that equation (3.1) can be represented in an equivalent form as a matrix mapping from a vector space to a vector space, with proper reshaping of tensor terms. In cases when system tensor \( A \) has some structure, treatment of the problem using the tensor representation can be more advantageous than using the conventional matrix formalism, that is explained in the next sections.
4 Tensor solvers

4.1 Direct tensor solvers, iterative tensor solvers, Krylov subspace tensor solvers

Here we introduce tensor solvers which can be explicitly applied to solve such tensor equations computationally. The most straightforward way to find the solution tensor and, if necessary, a tensor inverse - is based on use of a tensor extension of Gauss elimination or a tensor analogue of LU decomposition - both belonging to the class of direct tensor solvers. These methods can benefit from the explicit tensor structure of equation coefficients, which is typically manifested by handling multidimensional sub-blocks of nonzero coefficients. In many practical problems, however, tensor equations are so large that solving them using direct methods becomes prohibitive. In this instance, we propose the class of iterative tensor solvers. For example, one can use a tensor Jacobi solver which is based on the iterative computation of tensor multiplication and belongs to the class of stationary iterative solvers. The pseudocode of the algorithm and an actual software implementation are shown on Fig. 4.1.

Note that the presented object based implementation of the Jacobi solver does not use explicit indexing of tensor components. All information about indices is contained in tensor objects which are defined once at the construction stage. This is sufficient for performing further computations with automatic semantic analysis for optimizing the performance, and without complicating the solving process by explicit use of indices.

From the point of view of computational and storage requirements, the presented iterative solver is particularly attractive for application to tensor structured problems. As a basic example, consider the Poisson equation in three dimensions \( \nabla^2 u(x, y, z) = f(x, y, z) \) which after discretization on a uniform grid can be expressed by the following tensor equation

\[
\mathcal{A}^{x_1} \cdot U^{y_1 z_1} + \mathcal{B}^{y_1} \cdot U^{x_1 y_2 z_1} + \mathcal{C}^{z_1} \cdot U^{x_1 y_1 z} = F^{x_1 y_1 z_1}
\]

Here \( U \) is an unknown tensor, \( F \) is the observation tensor, \( \mathcal{A}, \mathcal{B}, \mathcal{C} \) are one-dimensional finite difference transformations which are equivalent to filters with impulse response dependent on the order of the Laplacian approximation. This decomposition allows very efficient computation of the tensor multiplication by performing sequential separable transformations along individual dimensions of the tensor \( U \). The separability renders the computation of the whole set of equation coefficients unnecessary, thus dramatically reducing storage requirements of the presented iterative algorithm (obviously, for such simple example, exploiting the tensor characteristics of the problem is also possible using the standard matrix approach with careful index bookkeeping).

Another type of iterative algorithms which are frequently used for solving large inverse problems, is the family of Krylov subspace solvers, which includes GMRES, CG, BICGSTAB and other solvers [23]. In our extension of this solver class to tensors, most of them can be expressed as an iterative application of the tensor multiplication (see Fig. 4.2) and thus profit from the
\[ \mathcal{R}^{x_1 y_1 z_1} = A_{x y z}^{x_1 y_1 z_1} \cdot U^{x y z} - B^{x_1 y_1 z_1} \]

for \( i = 0 \) until convergence

\[ U^{x y z} = U^{x y z} - \mathcal{R}^{x_1 y_1 z_1} \cdot E_{x y z} \]

\[ \mathcal{R}^{x_1 y_1 z_1} = A_{x y z}^{x_1 y_1 z_1} \cdot U^{x y z} - B^{x_1 y_1 z_1} \]

end

(a)

PROCEDURE TensorJacobi(A, B: Tensor;
threshold: Scalar
): Tensor;

VAR R, E, U: Tensor;

BEGIN

E := InvMainDiag(A, B);
R := A*U - B;

WHILE \( R^+R > \) threshold DO

U := U - R*E;
R := A*U - B;

END;

RETURN U;

END TensorJacobi;

(b)

VAR

w: World;
A, B, C: Tensor;

BEGIN

(* define a world with vector spaces *)

NEW(w);

w.DefineSpace('X', 128);
w.DefineSpace('Y', 129);
w.DefineSpace('Z', 130);

(* define system tensor *)

A := Tensors.Laplacian(w, "x\cdot1,x\cdot1,\ldots,y\cdot1,\ldots,z\cdot1,\ldots");

(* define right hand side *)

NEW(B, w, "x\cdot1,y\cdot1,\ldots,1,\ldots");
B.Fload("rhs.dat");

(* solve the problem *)

C := TensorJacobi(A, B, 1.0E-4);

\ldots

END

(c)

Fig. 4.1 (a) Pseudocode of tensor Jacobi iterator for three dimensions (\( E \) is the inverse of diagonal tensor constructed from main diagonal of \( A \)). (b) Actual implementation of solver for any number of dimensions using our tensor library designed in Tensor Oberon programming language, which offers algebraic operators and optimized implementations for the basic tensor operations. Here "*" and "+*" stand for tensor multiplication and inner product respectively. (c) A simple code example of using the solver.
same benefits discussed above for the tensor Jacobi iterator. In contrast to Jacobi solver which only converges well for a limited class of problems, Krylov solvers perform significantly better for the large majority of problems.

Fig. 4.2 presents a pseudocode and Oberon implementation of the tensor Conjugate Gradients (CG) algorithm applied to solve a 3D problem \( A_{xyz} \cdot C_{xyz} = B_{xyz} \).

\[ R_{xyz} = B_{xyz} - A_{xyz} \cdot C_{xyz} \]  
\[ P_{xyz} = R_{xyz} \]  
\[ \rho = \langle R_{xyz}, R_{xyz} \rangle \]  
\[ \alpha = \rho / \langle P_{xyz}, Q_{xyz} \rangle \]  
\[ C_{xyz} = C_{xyz} + \alpha \cdot P_{xyz} \]  
\[ R_{xyz} = R_{xyz} - \alpha \cdot Q_{xyz} \]  
\[ \rho_1 = \langle R_{xyz}, R_{xyz} \rangle \]  
\[ \rho = \rho_1 \]

**REPEAT**

\[ Q := A^*(P \cdot D); \]
\[ C := C + \alpha \cdot P \cdot D; \]
\[ R := R_1 - \alpha \cdot Q; \]
\[ rho1 := rho_1; \]
\[ rho := rho1; \]
\[ P := R + (rho1/\rho) \cdot P; \]

UNTIL \( \rho > \text{threshold} \)

**Fig. 4.2** Pseudocode and given side by side actual implementation of Conjugate Gradient iterator

### 4.2 Tensor Multigrid algorithms unify algebraic multigrid and geometric multiresolution

In the matrix domain, multigrid methods for solving linear system of equations are known for their fast convergence and computational efficiency. These methods perform iterative improvement of a solution approximation, based on smoothing of the solution error on multiple scales of the problem. Basically, there are two types of multigrid/multiresolution strategies: geometric multiresolution preserves spatial coherence in multidimensions by working on datasets at different resolutions but its formulation is often problem specific. **Algebraic** matrix multigrid algorithms (AMG) offer a 'black box' approach for solving matrix equations, but they rely on values of matrix coefficients only and risk neglecting data coherence, at a potential cost of degraded performance.

We have used tensor equations to express both approaches in a unified fashion. The proposed tensor multigrid algorithm (TMG) has an important advantage over AMG: in contrast to the matrix algorithm, which neglects multidimensionality and the structure of the problem, TMG unifies both concepts of geometric and algebraic multiresolution, by preserving and exploiting multidimensionality and spatial data coherence (see Fig. 4.3).
Fig. 4.3 shows pseudocode for a Tensor Algebraic Multigrid V-cycle algorithm applied to solve a 3D tensor problem $A^{xyz}_{x'y'z'} \cdot C_{xyz} = B_{x'y'z'}$. Problems in higher dimensions are handled in a similar way. Fig. 4.4 compares visually how AMG and TMG are applied to a problem of reconstruction of a two-dimensional image from a few arbitrarily taken samples, using non-uniform spline interpolation [3]. This example shows that performance of the AMG algorithm is significantly degraded due to data distortion, which is introduced at coarse matrix scales, whilst the TMG converges to a good approximation of the solution within a few iterations, due to its preservation of spatial coherence.

function $C^{xyz} = \text{TMGVCycle}(\text{scale}, A^{xyz}_{x'y'z'}, C^{xyz}, B^{xyz}_{x'y'z'})$

if scale $\neq$ last then
  $C^{xyz} = \text{Presmooth}(A^{xyz}_{x'y'z'}, C^{xyz}, B^{xyz}_{x'y'z'})$
  % get preliminary constructed system scale and % corresponding restriction/prolongation operators
  $[\hat{A}_{uvw}^{u'v'w'}, \hat{B}_{uvw}^{u'v'w'}, \hat{S}_{uvw}^{u'v'w'}, \hat{T}_{uvw}^{u'v'w'}, \hat{P}_{u}^{u'}, \hat{S}_{y}^{v'}, \hat{T}_{z}^{w'}] = \text{GetScale}(\text{scale})$
  % separable restriction of the residual
  $\hat{B}_{uvw}^{u'v'w'} = \hat{P}_{u}^{u'} \cdot \hat{S}_{y}^{v'} \cdot \hat{T}_{z}^{w'} \cdot (B^{xyz}_{x'y'z'} - A^{xyz}_{x'y'z'} \cdot C^{xyz})$
  $\hat{C}_{uvw}^{u'v'w'} = 0$
  $\hat{C}_{uvw}^{u'v'w'} = \text{TMGVCycle}(\text{scale} + 1, \hat{A}_{uvw}^{u'v'w'}, \hat{C}_{uvw}^{u'v'w'}, \hat{B}_{uvw}^{u'v'w'})$ % V-cycle on next scale
  $C^{xyz} = C^{xyz} + \hat{P}_{u}^{u'} \cdot \hat{S}_{y}^{v'} \cdot \hat{T}_{z}^{w'} \cdot \hat{C}_{uvw}^{u'v'w'}$ % coarse grid correction
  $C^{xyz} = \text{Postsmooth}(A^{xyz}_{x'y'z'}, C^{xyz}, B^{xyz}_{x'y'z'})$
else
  $C^{xyz} = \text{DirectSolve}(A^{xyz}_{x'y'z'}, B^{xyz}_{x'y'z'})$
end

Fig. 4.3 Pseudocode of a TMG V-cycle algorithm for three dimensions

5 Automatic tensor expression analysis for high-performance implementations

Because the high level tensor formulation contains the complete tensorial structure information of a complex mathematical problem, automatic expression analysis can be performed, resulting in automated software optimization and code generation. We have experimentally verified this aspect in our tensor library and have found that such automatic analysis is capable of optimizing code, with regard to computational and memory requirements, in both a problem-specific and hardware-specific manner. This result profits strongly from the commutativity of all tensor operations, the significant differentiating
feature over standard matrix formulations which are non-commutative with respect to matrix multiplication. Some aspects of such automated code generation have also been discussed in [4]. This particular topic is a promising area for future research.

6 Application of the framework to large real-world problems

Our framework was successfully applied to solve a large real-world computational problem - a spline-based global variational reconstruction [3] of a multidimensional signal from incomplete and spatially scattered measurements in four dimensions. The problem was originally formulated in terms of matrix algebra. In four dimensions, the matrices involved in the computations become extremely large, essentially prohibiting computation of the problem on current standard hardware. For example, for a moderate size of the reconstruction grid $128 \times 128 \times 128 \times 16$ we have to deal with a matrix which is represented by $7'514'444'528$ nonzero elements (in compressed block-band diagonal storage, 30 GBytes in single precision). Using our framework, we reformulated the problem in terms of tensors. The resulting tensor formulation helped to analyze the mathematical structure of the problem and to derive its decomposition in the form of a 1-rank tensor decomposition known as Canonical Decomposition (CANDECOMP) [11,14,19]. More details about proposed tensor formulation and solving algorithm can be found in our companion paper.

The identified tensorial structure allowed efficient computation of the tensor multiplication which therefore can be efficiently used within a tensor Krylov solver. Another important implication of the identified property of the tensor formulation, is a dramatic reduction of storage requirements. Our approach
does not require explicit storage either of the system tensor or its decom-
position, and thus the problem of size, discussed above (33'554'432 unknowns
parameters), for about 9’000’000 measurements, can be computed on current
inexpensive multi core computer equipped with only 2 GBytes of physical
memory in less than 60 minutes, surpassing the capability of a published,
matrix-based solving algorithm [3] for the same problem by far. The decom-
posability of the tensor multiplication allows convenient and complete paral-
lelization of computations using all currently available parallelism paradigms,
including Single Instruction Multiple Data (SIMD), Multi Core, Clusters of
PCs and General Purpose GPU (GPGPU) computing technology.

Note that parallelizability of tensor operations, in general, has proven to
be very beneficial: on Multi Core CPUs we have observed a speed increase
almost proportional to the number of cores; and on a recent graphics card (ATI
Radeon HD 4870 X2) an additional increase has been measured for specific
examples, of more than 10, compared to a Quad Core CPU.

7 Discussion

In this work we introduced a framework for computational solving of large ten-
sor structured problems. The proposed approach leads to a natural, dimensionality-
preserving formulation of tensor structured problems, and by maintaining the
multidimensional structure of the data, and the commutativity properties of
the framework, directly induces computationally efficient solving strategies
that can profit from automatic expression analysis, separability properties of
the tensor formulation, and the preservation of spatial coherence of the data,
to speed up convergence in tensor solvers as compared to their matrix coun-
terparts.

The chosen formalism based on Einstein notation together with introduced
commutativity of tensor multiplication, makes the framework well suited for
implementing a tensor programming language, offering self-optimized computa-
tions of tensor expressions by semantic analysis of their terms while avoiding
explicit use of tensor indexing in the actual implementations of solving pro-
grams. This was verified by implementing our own tensor library built on the
principles of the proposed framework.

The properties presented above distinguish our framework from one often
used in the field of tensor decompositions [27,17,16,11,14,11,19], but do not
limit its use for solving problems studied in that field.

The ongoing research shows that the framework is well suited for solving
problems of signal processing in higher dimensions, which have inherent tensor
structure. We are currently investigating its usefulness in problems from image
reconstruction, computer vision and fluid dynamics.
In summary, this high-level approach fits well into the landscape of increasing interest in tensors as a workhorse for elegant and efficient solving of those scientific problems which arise from multidimensional data.

### Table 7.1 Basic multidimensional data processing building blocks in separable tensor form

| Signal processing operator | Tensor expression | Corresponding implementation $^4$ |
|----------------------------|-------------------|-----------------------------------|
| Discrete convolution       | $F^{x_1 y_1 z_1} = E^{x_1} \cdot G^{y_1} \cdot H^{z_1} \cdot C^{xyz}$ | $F := E^*G^*H^*C$; |
| Finite difference $^5$     | $F^{x_1 y_1 z_1} = E^{x_1} \cdot C^{xyz}$ | $F := E^*C$; |
| Discrete Fourier transform | $F^{x_1 y_1 z_1} = E^{x_1} \cdot G^{y_1} \cdot H^{z_1} \cdot C^{xyz}$ | $F := E^*G^*H^*C$; |
| Rotation                   | $F^{x_1 y_1 z_1} = D^{x_1} \cdot (E^{x_1} \cdot G^{y_1} \cdot H^{z_1} \cdot C^{xyz})$ | $F := D^*E^*G^*H^*C$; |
| Upsampling/downsampling    | $F^{x_1 y_1 z_1} = E^{x_1} \cdot G^{y_1} \cdot H^{z_1} \cdot C^{xyz}$ | $F := E^*G^*H^*C$; |

Objects C,D,E,F,G,H correspond respectively to C,D,E,F,G,H from tensor expressions; $^*$ denotes the tensor product

The tensor representation of finite difference is the base for derivative related operators such as gradient, divergence, curl and Laplacian.

### Table 7.2 Large scientific problems suited for solution by computational Tensor Algebra

| Computational Application | Scientific Field |
|----------------------------|------------------|
| Multilinear data models using tensor decompositions (e.g. CANDECOMP, TUCKER, HOSVD): | Signal Processing |
| - Pattern recognition $^{[20,29]}$ | Computer Vision |
| - Data compression $^{[13]}$ | Data Mining |
| - Independent Component Analysis $^{[6,15]}$ | Chemistry |
| - Signal filtering $^{[20]}$ | Neuroscience |
| - Modeling of fluorescence data $^{[1]}$ | |
| Solving inverse multidimensional problems: | |
| - Least squares problems $^{[3,21]}$ | Signal Processing |
| - Differential equations (Poisson, Navier-Stokes, Finite Element Methods) $^{[18,9]}$ | Computer Vision |
| - Integral equations $^{[8]}$ | Machine Learning |
| - Modeling of properties of complex systems consisting of many interacting elements expressed by tensor expressions: | Fluid Dynamics |
| - Modeling of electronic and optical properties of molecules and their interactions $^{[25,22]}$ | Chemistry |
| | Electromagnetism |
| | Computational Physics |
| | Quantum Chemistry |
| | Computational Chemistry |
| | Material Science |

$^4$ Objects C,D,E,F,G,H correspond respectively to C,D,E,F,G,H from tensor expressions; $^*$ denotes the tensor product

$^5$ The tensor representation of finite difference is the base for derivative related operators such as gradient, divergence, curl and Laplacian.
A APPENDIX

A.1 Dual vectors spaces, contravariant and covariant mechanisms of transformation

Let \( V \) be a real vector space with finite number of dimensions \( N \). We designate by \( V^* \) unique vector space of same dimensionality that is dual in respect to \( V \). Any element \( t^* \in V^* \) is a linear map \( V \to \mathbb{R} \)

\[
(t^*, t) \equiv t^*(t) \in \mathbb{R} \tag{A.1}
\]

For a given base \( e_v \) of \( V \) transformations to a new base \( \hat{e}_{v_1} \) and vice versa are defined by

\[
\hat{e}_{v_1} = \sum_{v=1}^{N} P_{v_1}^v \cdot e_v, \quad e_{v_2} = \sum_{v_1=1}^{N} S_{v_2}^{v_1} \cdot \hat{e}_{v_1} \tag{A.2}
\]

where \( P_{v_1}^v \) and \( S_{v_2}^{v_1} \) are direct and indirect base transformations respectively. A vector from \( V \) given by

\[
\sum_{v=1}^{N} T^v \cdot e_v
\]

according to \( \text{(A.2)} \) in a new coordinate system is represented by components

\[
\hat{T}^v_{v_1} = \sum_{v_1=1}^{N} S_{v_1}^{v_1} \cdot T^v
\]

Components of such vectors which transform indirectly in respect to transformation of the base are called contravariant.

For the base \( e_v \) of \( V \) and dual base \( e^*_v \) the following equation is satisfied

\[
\langle e^*_v, e_v \rangle \equiv \delta^v_v = \begin{cases} 1, & \text{if } v_1 = v \\ 0, & \text{if } v_1 \neq v \end{cases} \tag{A.4}
\]

where \( \delta^v_v \) is Kronecker delta. Thus the dual base \( e^*_v \) transforms according to

\[
\hat{e}^v_{v_1} = \sum_{v_1=1}^{N} S_{v_1}^{v_1} \cdot e^v, \quad e^v_{v_2} = \sum_{v_2=1}^{N} P_{v_2}^{v_2} \cdot \hat{e}^v_{v_2}
\]

\[
\tau_{v_2} = \sum_{v_1=1}^{N} P_{v_2}^{v_1} \cdot \tau_{v_1}
\]

Components of such vectors are called covariant.

A.2 Generalized definition of a tensor

**Definition A.1** Let ordered set of real vector spaces \( U_1, \ldots, U_P, \ V_1, \ldots, V_Q \) with finite dimensions \( I_1, \ldots, I_P, \ J_1, \ldots, J_Q \) and their dual vector space \( U_1^*, \ldots, U_P^*, \ V_1^*, \ldots, V_Q^* \) be given. By identifying \((U^*_i)^* \) with \( U_i \) we define every vector \( u_i \in U_i \) to be a linear map \( U_i^* \to \mathbb{R} \) given by

\[
u_i(u_i^*) \equiv (u_i^*, u_i) \in \mathbb{R} \tag{A.7}
\]

for arbitrary \( u_i^* \in U_i^* \), where \( (, ) \) denotes the inner product. With \((P + Q)\) vectors \( u_i \in U_1, \ldots, u_P \in U_P, \ v_i^* \in V_1^*, \ldots, v_Q^* \in V_Q^* \) let the element denoted \( T = u_1 \times \cdots \times u_P \times v_1^* \times \cdots \times v_Q^* \) be a \((P + Q)\)-linear map from \( U_1 \times \cdots \times U_P \times V_1^* \times \cdots \times V_Q^* \to \mathbb{R} \) defined by
\[ \mathbf{u}_1 \times \cdots \times \mathbf{u}_P \times \mathbf{v}^*_1 \times \cdots \times \mathbf{v}^*_Q (a^*_1, \ldots, a^*_P, b_1, \ldots, b_Q) = \\
(a^*_1, \mathbf{u}_1) \cdots (a^*_P, \mathbf{u}_P) (\mathbf{v}^*_1, b_1) \cdots (\mathbf{v}^*_Q, b_Q) \] (A.8)

where \( a^*_i, b_j \) are arbitrary vectors in \( U^*_i \) and \( V_j \) respectively. The element \( T \) is termed a \((P+Q)\)-th order decomposed tensor, \( P \)-times contravariant and \( Q \)-times covariant. The space generated by all linear combinations of decomposed tensors is termed the tensor product space. Any arbitrary tensor can be represented as a weighted sum of decomposed tensors [14][19][15]. This definition is compatible with, and extends [17][21].

A.3 Tensor notation

To each dimension of the physical space we assign a vector space with a given dimensionality. For example for 3-dimensional physical space we define vector spaces \( X, Y, Z \) with sizes \( N_X, N_Y, N_Z \). In such vector spaces one can define multiple coordinate systems related to each other by transformations discussed above. Components of a tensor in some tensor product space are designated as an array with multiple indices. Each index in the designation has direct correspondence to a dimension of the physical space and thus to one of the defined vector spaces. For example for 3-dimensional case a tensor which is an element of \( X \times Y \times Z \) can be designated by \( T^{x_1y_1z_1} \). Subindices \( i, j, k \) are used for distinguishing between different coordinate systems.

A.4 Elementwise tensor operations

Linearity of the defined tensor product space implies definition of the following elementwise tensor operations such as tensor addition, subtraction and multiplication by a scalar:

\[ A^{x_1y_1z_1} + B^{x_1y_1z_1} = C^{x_1y_1z_1} \] (A.9)
\[ A^{x_1y_1z_1} - B^{x_1y_1z_1} = D^{x_1y_1z_1} \] (A.10)
\[ \lambda \cdot A^{x_1y_1z_1} = E^{x_1y_1z_1} \] (A.11)

With introduced constraint of ordered vector spaces all properties of these operations such as associativity and commutativity remain unchanged.

A.5 Kronecker delta

Kronecker delta presented in expression (A.4) is a second order tensor which is equivalent to the identity transformation. Mixed version of the tensor applied to components of a contravariant or covariant first order tensor (vector) does not introduce changes

\[ \delta^{x_1} \cdot \mathbf{T}^x = \mathbf{T}^{x_1} \equiv \mathbf{T}^x \] (A.12)
\[ \delta_{x_1} \cdot \mathbf{U}_{x_1} = \mathbf{U}_x \equiv \mathbf{U}_{x_1} \] (A.13)

Covariant or contravariant versions of the Kronecker delta change variance of tensor indices, but do not change values of tensor components

\[ \delta^{x_1} \cdot \mathbf{T}_x = \mathbf{T}_{x_1} \equiv \mathbf{T}_x \] (A.14)
\[ \delta_{x_1} \cdot \mathbf{U}_{x_1} = \mathbf{U}^x \equiv \mathbf{U}^{x_1} \] (A.15)
Note that here indices $x$ and $x_1$ correspond to identical coordinate systems. In the same way Kronecker delta can be applied along some dimension of a higher order tensor

$$\delta^x_{x_1} \cdot T^{xyz} \equiv \delta^y_{y_1} \cdot T^{xyz} \equiv \delta^z_{z_1} \cdot T^{xyz} \equiv T^{xyz} \quad (A.16)$$

The tensor multiplication of Kronecker deltas for different vector spaces forms multi-dimensional identity transformation

$$\delta^x_{x_1} \cdot \delta^y_{y_1} \cdot \delta^z_{z_1} \equiv T^{xyz} \quad (A.17)$$

$$\delta^x_{x_1} \cdot T^{xyz} \equiv T^{x_1y_1z_1} \equiv T^{xyz} \quad (A.18)$$

A.6 Inner product

the inner product of two third order Euclidean tensors $A^{xyz}$ and $B^{xyz}$ is defined by

$$\langle A, B \rangle = (A^{xyz} \cdot \delta_{x_1y_1z_1}) \cdot (B^{xyz} \cdot \delta_{x_1y_1z_1}) = A^{x_1y_1z_1} \cdot B^{x_1y_1z_1} \quad (A.19)$$

At the same time using the language of elementwise products the inner product can be expressed as

$$\langle A, B \rangle = (A^{xyz} \cdot B^{xyz}) \cdot (\delta_{x_1y_1z_1}) \cdot (\delta_{x_1y_1z_1}) = C^{x_1y_1z_1} \cdot I_{x_1y_1z_1} \quad (A.20)$$

where $I_{x_1y_1z_1}$ is a tensor with all components equal to one, which can be easily checked based on the properties of Kronecker delta.

Note that in general case of non-Euclidean spaces the inner product is defined with the use of the metric tensor which for Euclidean case reduces to the Kronecker delta.

A.7 Tensor transposition

In classical settings transposition of a tensor is defined by changing positions of tensor indices. But in our framework the order of indices is unique according to a predefined order of vector spaces. Thus patterns like $A^T A$ from matrix normal equations correspond to the tensor multiplication with change of variance by the Kronecker delta in Euclidean spaces or the metric tensor in general case.

A.8 Differentiation in respect to a tensor

When dealing with an optimization problem, differentiation in respect to the optimization parameter may be required. Consider an example of differentiating a tensor valued function of the form $f(U) = A^x_{y_1z_1} \cdot U^{xyz}$

$$\frac{\partial}{\partial U} f(U) = \frac{\partial}{\partial U} (A^x_{y_1z_1} \cdot U^{xyz}) = A^x_{y_1z_1} \cdot \left( \frac{\partial U^{xyz}}{\partial U^{x_2y_2z_2}} \right) \quad (A.21)$$

where indices $(x, y, z)$ and $(x_2, y_2, z_2)$ correspond to identical coordinate systems. Using tensor transformational properties it is straightforward to show that

$$\frac{\partial U^{xyz}}{\partial U^{x_2y_2z_2}} = \delta^{xyz}_{x_2y_2z_2} \quad (A.22)$$

Thus we have

$$\frac{\partial}{\partial U} f(U) = A^x_{y_1z_1} \cdot \delta^{xyz}_{x_2y_2z_2} = A^{x_1y_1z_1} \equiv A^{x_1y_1z_1} \quad (A.23)$$

In a similar way one can compute derivative of more complex scalar and tensor valued functions.
References

1. Acar, E., Yener, B.: Unsupervised Multiway Data analysis: A Literature Survey. IEEE Trans. on Knowl. and Data Eng. 21(1), 6–20 (2009). DOI http://dx.doi.org/10.1109/TKDE.2008.112
2. Aldroubi, A., Unser, M.: Wavelets in Medicine and Biology. CRC Press, Boca Raton FL, USA (1996). 616 p.
3. Arigovindan, M., Suchling, M., Hunziker, P., Unser, M.: Variational Image Reconstruction from Arbitrarily Spaced Samples: A Fast Multiresolution Spline Solution. IEEE Transactions on Image Processing 14(4), 450–460 (2005). DOI 10.1109/TIP.2004.841203. URL http://bigwww.epfl.ch/publications/arigovindan0501.ps, http://bigwww.epfl.ch/publications/arigovindan0501.html
4. Baumgartner, G., Auer, E., Bernholdt, D.E., Bibireata, A., Cociorva, D., Gao, X., Krishnan, S., Harrison, R.J., Chung Lam, C., Lu, Q., Nooijen, M.: Synthesis of High-Performance Parallel Programs for a Class of Ab Initio Quantum Chemistry Models. In: Proceedings of the IEEE, pp. 276–292 (2005)
5. Blahut, R.E.: Fast Algorithms for Digital Signal Processing. Addison-Wesley (1985)
6. Comon, P.: Tensor decompositions, state of the art and applications. IMA Conference Mathematics in Signal Processing, Warwick, UK (2000)
7. Einstein, A.: The Foundation of the General Theory of Relativity. In: The Collected Papers of Albert Einstein, vol. 6, pp. 146–200. Princeton University Press (1997)
8. Elden, L.: Multi-linear mappings, SVD, HOSVD, and the numerical solution of ill-conditioned tensor least squares problems. In: Workshop on Tensor Decompositions and Applications TDA05 (2005)
9. Gavriljuk, I.P., Hackbusch, W., Khoromskij, B.N.: Hierarchical tensor-product approximation to the inverse and related operators for high-dimensional elliptic problems. Computing 74(2), 131–157 (2005). DOI http://dx.doi.org/10.1007/s00607-004-0086-y
10. Guoan, B., Yonghong, Z.: Transforms and fast algorithms for signal analysis and representations. Boston : Birkhauser (2004)
11. Harshman, R.A.: Foundations of the PARAFAC procedure: Model and conditions for an explanatory multi-mode factor analysis. UCLA Working Papers in phonetics 16, pp. 1–84 (1970)
12. Heinbockel, J.H.: Introduction to tensor calculus and continuum mechanics. Trafford Publishing, Norfolk, Virginia (2001)
13. Hongcheng, W., Ahuja, N.: Compact representation of multidimensional data using tensor rank-one decomposition. Pattern Recognition, 2004 . ICPR 2004. Proceedings of the 17th International Conference on 1, 44–47 Vol.1 (2004). DOI 10.1109/ICPR.2004.1334001
14. Kolda, T.G., Bader, B.W.: Tensor Decompositions and Applications. SIAM Review 51(3) (2009 (to appear))
15. Lathauwer, L.D., Moor, B.D.: From Matrix to Tensor : Multilinear Algebra and Signal Processing. Mathematics in Signal Processing IV, McWhirter J., ed. pp. 1–15 (1998). Selected papers presented at 4th IMA Int. Conf. on Mathematics in Signal Processing
16. Lathauwer, L.D., Moor, B.D., Vandewalle, J.: A Multilinear Singular Value Decomposition. SIAM J. Matrix Anal. Appl. 21(4), 1253–1278 (2000). DOI http://dx.doi.org/10.1137/S0895479896305096
17. Leibovici, D., Sabatier, R.: A Singular Value Decomposition of a k-Way Array for a Principal Component Analysis of Multiway Data, PTA-k. Linear Algebra and its Applications 269, 307–329 (1998). DOI doi:10.1016/S0024-3795(97)81516-9. URL http://www.ingentaconnect.com/content/els/00243795/1998/000000269/00000001/art81516
18. Lynch, R.E., Rice, J.R., Thomas, D.H.: Tensor product analysis of partial difference equations. Bull. Amer. Math. Soc. 70, 3, 378–384 (1964)
19. Martin, C.M.: Tensor Decompositions Workshop Discussion Notes (2004). URL http://www.aimath.org/WWN/tensordecomp/tensorsdecomp.pdf
20. Muti, D., Bourennane, S.: Multidimensional signal processing using lower-rank tensor approximation. Acoustics, Speech, and Signal Processing, 2003. Proceedings. (ICASSP ’03). 2003 IEEE International Conference on 3, III–457–60 vol.3 (2003). DOI 10.1109/ICASSP.2003.1199510
21. Pereyra, V., Scherer, G.: Efficient Computer Manipulation of Tensor Products with Applications to Multidimensional Approximation. Mathematics of Computation 27(123), 595–605 (1973). URL http://www.jstor.org/stable/2005663
22. Raghavachari, K.: Electron Correlation Techniques in Quantum Chemistry: Recent Advances. Annual Review of Physical Chemistry 42, 615–642 (1991)
23. Saad, Y., van der Vorst, H.A.: Iterative solution of linear systems in the 20th century. J. Comput. Appl. Math. 123(1-2), 1–33 (2000). DOI http://dx.doi.org/10.1016/S0377-0427(00)00412-X
24. Savas, B., Elden, L.: Handwritten digit classification using higher order singular value decomposition. Pattern Recognition 40(3), 993 – 1003 (2007). DOI DOI:10.1016/j.patcog.2006.08.004. URL http://www.sciencedirect.com/science/article/B6V14-4M4CVHS-1/2/45630160cd85eb0532d9a5cf03e3c8fd
25. Schmidt, M.W., Baldridge, K.K., Boatz, J.A., Elbert, S.T., Gordon, M.S., Jensen, J.H., Koseki, S., Matsunaga, N., Nguyen, K.A., Su, S., Windus, T.L., Dupuis, M., Montgomery, J.A.: General atomic and molecular electronic structure system. Journal of Computational Chemistry 14, 11, 1347–1363 (1993). DOI 10.1002/jcc.540141112. URL http://dx.doi.org/10.1002/jcc.540141112
26. Smilde A. Bro, R., Geladi, P.: Multi-Way Analysis: Applications in the Chemical Sciences. Wiley, West Sussex, England (2004)
27. Tucker, L.R.: Some mathematical notes on three-mode factor analysis. Psychometrika 31, 279–311 (1966). DOI 10.1007/BF02289464. URL http://www.springerlink.com/content/b7z551g73474n136
28. Vasilescu, M., Terzopoulos, D.: Multilinear image analysis for facial recognition. Pattern Recognition, 2002. Proceedings. 16th International Conference on 2, 511–514 vol.2 (2002). DOI 10.1109/ICPR.2002.1048350