Springer Series in Computational Mathematics 42

Wolfgang Hackbusch

Tensor Spaces and Numerical Tensor Calculus

Springer

Springer Series in Computational Mathematics

42

For further volumes:
http://www.springer.com/series/797

Wolfgang Hackbusch

Tensor Spaces and Numerical Tensor Calculus

Springer

Wolfgang Hackbusch
Max-Planck-Institute
for Mathematics in the Sciences
Leipzig
Germany

ISSN 0179-3632
ISBN 978-3-642-28026-9 e-ISBN 978-3-642-28027-6
DOI 10.1007/978-3-642-28027-6
Springer Heidelberg Dordrecht London New York

Library of Congress Control Number: 2012933366

Mathematics Subject Classification (2010): 15A69, 35C99, 44A35, 46A32, 46B28, 47A80, 65F99 65N99 65L99 65N22 65N99 65Z05

Printed on acid-free paper

Springer is part of Springer Science+Business Media (www.springer.com)

Dedicated to my grandchildren
Alina and Daniel

Preface

Large-scale problems have always been a challenge for numerical computations. An example is the treatment of fully populated $n \times n$ matrices, when n^2 is close to or beyond the computer's memory capacity. Here, the technique of hierarchical matrices can reduce the storage and the cost of numerical operations from $O(n^2)$ to almost $O(n)$.

Tensors of order (or spatial dimension) d can be understood as d-dimensional generalisations of matrices, i.e., arrays with d discrete or continuous arguments. For large $d \geq 3$, the data size n^d is far beyond any computer capacity. This book concerns the development of compression techniques for such high-dimensional data via suitable data sparse representations. Just as the hierarchical matrix technique was based on a successful application of the low-rank strategy, in recent years, related approaches have been used to solve high-dimensional tensor-based problems numerically. The results are quite encouraging, at least for data arising from suitably smooth problems, and even some problems of size $n^d = 1000^{1000}$ have become computable.

The methods, which can be applied to these multilinear problems, are black box-like. In this aspect they are similar to methods used in linear algebra. On the other hand, most of the methods are approximate (computing suitably accurate approximations to quantities of interest) and in this respect they are similar to some approaches in analysis. The crucial key step is the construction of an efficient new tensor representation, thus overcoming the drawbacks of the traditional tensor formats. In 2009 a rapid progress could be achieved by introducing the hierarchical format as well as the TT format for the tensor representation. Under suitable conditions these formats allow a stable representation and a reduction of the data size from n^d to $O(dn)$. Another recent advancement is the so-called tensorisation technique, which may replace the size n by $O(\log n)$. Altogether, there is the hope that problems of size h^d can be reduced to size $O(d \log(n)) = O(\log(n^d))$, i.e., we reduce the problems to *logarithmical size*.

It turned out that some of the raw material for the methods described in this book was already known in the literature belonging to other (applied) fields outside of mathematics, such as chemistry. However, the particular language used to describe this material, combined with the fact that the algorithms (although potentially of general interest) were given names relating them only to a particular application, prevented the dissemination of the methods to a wider audience.

One of the aims of this monograph is to introduce a more mathematically-based treatment of this topic. Through this more abstract approach, the methods can be better understood, independently of the physical or technical details of the application.

The material in this monograph has been used for as the basis for a course of lectures at the University Leipzig in the summer semester of 2010.

The author's research at the Max-Planck Institute of Mathematics in the Sciences has been supported by a growing group of researchers. In particular we would like to mention: B. Khoromskij, M. Espig, L. Grasedyck, and H.J. Flad. The help of H.J. Flad was indispensable for bridging the terminological gap between quantum chemistry and mathematics. The research programme has also benefited from the collaboration between the group in Leipzig and the group of E. Tyrtyshnikov in Moscow. E. Tyrtyshnikov and I. Oseledets have delivered important contributions to the subject. A further inspiring cooperation[1] involves R. Schneider (TU Berlin, formerly University of Kiel). The author thanks many more colleagues for stimulating discussions.

The author also wishes to express his gratitude to the publisher Springer for their friendly cooperation.

Leipzig, October 2011 *Wolfgang Hackbusch*

[1] The groups in Leipzig and Berlin thank the Germany Research Society (DFG) for financial support within the priority program 1324 (Schwerpunktprogramm “Extraktion quantifizierbarer Information aus komplexen Systemen”). The Russian partner has been supported by the Russian Foundation for Basic Research RFBR.

Contents

List of Symbols and Abbreviations

Symbols

$[a\ b\ \ldots]$	aggregation of vectors $a, b \in \mathbb{K}^I, \ldots$ into a matrix of size $I \times J$
$[A\ B\ \ldots]$	aggregation of matrices $A \in \mathbb{K}^{I\times J_1}$, $B \in \mathbb{K}^{I\times J_2}, \ldots$ into a matrix of size $I \times (J_1 \cup J_2 \cup \ldots)$
$\lceil\cdot\rceil$	smallest integer $\geq \cdot$
$\lfloor\cdot\rfloor$	largest integer $\leq \cdot$
$\langle\cdot,\cdot\rangle$	scalar product; in $\mathbb{K}^I$ usually the Euclidean scalar product; cf. §2.1, §4.4.1
$\langle\cdot,\cdot\rangle_\alpha$	partial scalar product; cf. (4.66)
$\langle\cdot,\cdot\rangle_H$	scalar product of a (pre-)Hilbert space H
$\langle\cdot,\cdot\rangle_{\mathrm{HS}}$	Hilbert-Schmidt scalar product; cf. Definition 4.117
$\langle\cdot,\cdot\rangle_j$	scalar product of the (pre-)Hilbert space V_j from $\mathbf{V} = \bigotimes_{j=1}^d V_j$
$\langle\cdot,\cdot\rangle_{\mathsf{F}}$	Frobenius scalar product of matrices; cf. (2.10)
$\#$	cardinality of a set
$\rightharpoonup$	weak convergence; cf. §4.1.7
$\bullet\vert_{\tau\times\sigma}$	restriction of a matrix to the matrix block $\tau \times \sigma$; cf. §1.7
$\bullet^\perp$	orthogonal complement, cf. §4.4.1
$\bullet^{\mathsf{H}}$	Hermitean transpose of a matrix or vector
$\bullet^{\mathsf{T}}$	transpose of a matrix or vector
$\bullet^{-\mathsf{T}}, \bullet^{-\mathsf{H}}$	inverse matrix of $\bullet^{\mathsf{T}}$ or $\bullet^{\mathsf{H}}$, respectively
$\overline{\bullet}$	either complex-conjugate value of a scalar or closure of a set
$\times$	Cartesian product of sets: $A \times B := \{(a, b) : a \in A, b \in B\}$
$\times_{j=1}^d$	d-fold Cartesian product of sets
$\times_j$	j-mode product, cf. Footnote 6 on page 5; not used here
$\star$	convolution; cf. §4.6.5
$\wedge$	exterior product; cf. §3.5.1
$\odot$	Hadamard product; cf. (4.72a)
$\oplus$	direct sum; cf. footnote on page 21
$\otimes^d$	d-fold tensor product; cf. Notation 3.23

$v \otimes w$, $\bigotimes_{j=1}^{d} v^{(j)}$ tensor product of two or more vectors; cf. §3.2.1
$V \otimes W$, $\bigotimes_{j=1}^{d} V_j$ tensor space generated by two or more vector spaces; cf. §3.2.1
$V \otimes_a W$, ${}_a\bigotimes_{j=1}^{d} V_j$ algebraic tensor space; cf. (3.11) and §3.2.4
$V \otimes_{\|\cdot\|} W$, ${}_{\|\cdot\|}\bigotimes_{j=1}^{d} V_j$ topological tensor space; cf. (3.12); §4.2
$\bigotimes_{j \neq k}$ cf. (3.21b)
$\subset$ the subset relation $A \subset B$ includes the case $A = B$
$\dot{\cup}$ disjoint union
$\sim$ equivalence relation; cf. §3.1.3, §4.1.1
$\bullet \cong \bullet$ isomorphic spaces; cf. §3.2.5
$\bullet \leq \bullet$ semi-ordering of matrices; cf. (2.14)
$\|\cdot\|$ norm; cf. §4.1.1
$\|\cdot\|^*$ dual norm; cf. Lemma 4.18
$\|\cdot\|_2$ Euclidean norm of vector or tensor (cf. (2.12) and Example 4.126) or spectral norm of a matrix (cf. (2.13))
$\|\cdot\|_\mathsf{F}$ Frobenius norm of matrices; cf. (2.9)
$\|\cdot\|_{\mathrm{HS}}$ Hilbert-Schmidt norm; cf. Definition 4.117
$\|\cdot\|_{\mathrm{SVD},p}$ Schatten norm; cf. (4.17)
$\|\cdot\|_X$ norm of a space X
$\|\cdot\|_{X \leftarrow Y}$ associated matrix norm (cf. (2.11) or operator norm (cf. (4.6a))
$\|\cdot\|_1 \lesssim \|\cdot\|_2$ semi-ordering of norms; cf. §4.1.1
$\|\cdot\|_{\wedge(V,W)}$, $\|\cdot\|_\wedge$ projective norm; cf. §4.2.4
$\|\cdot\|_{\vee(V,W)}$, $\|\cdot\|_\vee$ injective norm; cf. §4.2.7

Greek Letters

α often a subset of the set D of directions (cf. (5.3a,b)) or vertex of the tree T_D (cf. Definition 11.2)
α^c complement $D \backslash \alpha$; cf. (5.3c)
α_1, α_2 often sons of a vertex $\alpha \in T_D$; cf. §11.2.1
δ_{ij} Kronecker delta; cf. (2.1)
$\boldsymbol{\rho}$ tuple of TT ranks; cf. Definition 12.1
$\rho(\cdot)$ spectral radius of a matrix; cf. §4.6.6
$\rho_{\mathrm{xyz}}(\cdot)$ tensor representation by format 'xyz'; cf. §7.1
ρ_{frame} general tensor subspace format; cf. (8.13c)
ρ_{HOSVD} HOSVD tensor subspace format; cf. (8.26)
ρ_{HTR} hierarchical format; cf. (11.28)
$\rho_{\mathrm{HTR}}^{\mathrm{HOSVD}}$ hierarchical HOSVD format; cf. Definition 11.36
$\rho_{\mathrm{HTR}}^{\mathrm{orth}}$ orthonormal hierarchical format; cf. (11.38)
$\rho_{\mathrm{HTR}}^{\mathrm{tens}}$ TT format for tensorised vectors; cf. (14.5a)
ρ_{hybr}, $\rho_{\mathrm{orth}}^{\mathrm{hybr}}$, $\rho_{\mathrm{r\text{-}term}}^{\mathrm{hybr}}$ hybrid formats; cf. §8.2.4
ρ_j TT rank; cf. (12.1a) and Definition 12.1
ρ_{orth} orthonormal tensor subspace format; cf. (8.8b)

$\rho_{\text{r-term}}$ r-term format; cf. (7.7a)
ρ_{sparse} sparse format; cf. (7.5)
ρ_{TS} general tensor subspace format; cf. (8.6c)
ρ_{TT} TT format; cf. (12.7)
$\sigma(\cdot)$ spectrum of a matrix; cf. §4.6.6
σ_i singular value of the singular value decomposition; cf. (2.19a), (4.59)
Σ diagonal matrix of the singular value decomposition; cf. (2.19a)
φ, ψ often linear mapping or functional (cf. §3.1.4)
Φ, Ψ often linear mapping or operator (cf. §4.1.4)
Φ' dual of Φ; cf. Definition 4.20
Φ^* adjoint of Φ; cf. Definition 4.113

Latin Letters

$\mathbf{a}$ coefficient tensor, cf. Remark 3.29
$A, B, \ldots, A_1, A_2, \ldots$ often used for linear mapping (from one vector space into another one). This includes matrices.
$\mathbf{A}, \mathbf{B}, \mathbf{C}, \ldots$ tensor products of operators or matrices
$A^{(j)}$ mapping from $L(V_j, W_j)$, j-th component in a Kronecker product
$\mathcal{A}(V)$ tensor algebra generated by V; cf. (3.43)
$\mathfrak{A}(V)$ antisymmetric tensor space generated by V; cf. Definition 3.62
Arcosh area [inverse] hyperbolic cosine: $\cosh(\text{Arcosh}(x)) = x$
$b_i^{(j)}, \mathbf{b}_i^{(\alpha)}$ basis vectors; cf. (8.5a), (11.20a)
$B, B_j, \mathbf{B}_\alpha$ basis (or frame), $B_j = \left[b_1^{(j)}, \ldots, b_r^{(j)}\right]$, cf. (8.5a-d); in the case of tensor spaces: $\mathbf{B}_\alpha = \left[\mathbf{b}_1^{(\alpha)}, \ldots, \mathbf{b}_{r_\alpha}^{(\alpha)}\right]$, cf. (11.20a)
$c_0(I)$ subset of $\ell^\infty(I)$; cf. (4.4)
$c_{ij}^{(\alpha,\ell)}$ coefficients of the matrix $C^{(\alpha,\ell)}$; cf. (11.24)
$\mathbb{C}$ field of complex numbers
$C(D), C^0(D)$ bounded, continuous functions on D; cf. Example 4.8
$\mathbf{C}_\alpha$ tuple $(C^{(\alpha,\ell)})_{1\le\ell\le r_\alpha}$ of $C^{(\alpha,\ell)}$ from below; cf. (11.27)
$C^{(\alpha,\ell)}$ coefficient matrix at vertex α characterising the basis vector $\mathbf{b}_\ell^{(\alpha)}$; cf. (11.24)
$\mathfrak{C}_j, \mathfrak{C}_\alpha$ contractions; cf. Definition 4.130
$C_N(f,h), C(f,h)$ sinc interpolation; cf. Definition 10.31
d order of a tensor; cf. §1.1.1
D set $\{1, \ldots, d\}$ of directions; cf. (5.3b)
$\mathfrak{D}_\delta$ analyticity stripe; cf. (10.38)
$depth(\cdot)$ depth of a tree; cf. (11.7)
$\det(\cdot)$ determinant of a matrix
$\text{diag}\{\ldots\}$ diagonal matrix with entries ...
$\dim(\cdot)$ dimension of a vector space
$e^{(i)}$ i-th unit vector of $\mathbb{K}^I$ ($i \in I$); cf. (2.2)

$E_N(f,h), E(f,h)$ sinc interpolation error; cf. Definition 10.31
$E_r(\cdot)$ exponential sum; cf. (9.27a)
$\mathcal{E}_\rho$ regularity ellipse; cf. §10.4.2.2
$\mathcal{F}(W,V)$ space of finite rank operators; cf. §4.2.13
$G(\cdot)$ Gram matrix of a set of vectors; cf. (2.16), (11.35)
$H, H_1, H_2, \ldots$ (pre-)Hilbert spaces
$\mathbf{H}(\mathfrak{D}_\delta)$ Banach space from Definition 10.33
$H^{1,p}(D)$ Sobolev space; cf. Example 4.41
$HS(V,W)$ Hilbert-Schmidt space; cf. Definition 4.117
id identity mapping
$i, j, k, \ldots$ index variables
$\mathbf{i}, \mathbf{j}, \mathbf{k}$ multi-indices from a product index set $\mathbf{I}$ etc.
I identity matrix or index set
$\mathcal{I}, \mathcal{I}_{[a,b]}$ interpolation operator; cf. §10.4.3
$I, J, K, I_1, I_2, \ldots, J_1, J_2, \ldots$ often used for index sets
$\mathbf{I}, \mathbf{J}$ index sets defined by products $I_1 \times I_2 \times \ldots$ of index sets
j often index variable for the directions from $\{1, \ldots, d\}$
$\mathbb{K}$ underlying field of a vector space; usually $\mathbb{R}$ or $\mathbb{C}$
$\mathcal{K}(W,V)$ space of compact operators; cf. §4.2.13
$\ell(I)$ vector space $\mathbb{K}^I$; cf. Example 3.1
$\ell_0(I)$ subset of $\ell(I)$; cf. (3.2)
$\ell^p(I)$ Banach space from Example 4.5; $1 \le p \le \infty$
$level$ level of a vertex of a tree, cf. (11.6)
L often depth of a tree, cf. (11.7)
L lower triangular matrix in Cholesky decomposition; cf. §2.5.1
$\mathcal{L}(T)$ set of leaves of the tree T; cf. (11.9)
$L(V,W)$ vector space of linear mappings from V into W; cf. §3.1.4
$\mathcal{L}(X,Y)$ space of continuous linear mappings from X into Y; cf. §4.1.4
$L^p(D)$ Banach space; cf. Example 4.7; $1 \le p \le \infty$
$\mathcal{M}_\alpha, \mathcal{M}_j$ matricisation isomorphisms; cf. Definition 5.3
n, n_j often dimension of a vector space V, V_j
$\mathbb{N}$ set $\{1, 2, \ldots\}$ of natural numbers
$\mathbb{N}_0$ set $\mathbb{N} \cup \{0\} = \{0, 1, 2, \ldots\}$
$\mathcal{N}(W,V)$ space of nuclear operators; cf. §4.2.13
N_{xyz} arithmetical cost of 'xyz'
$N_{\mathrm{mem}}^{\mathrm{xyz}}$ storage cost of 'xyz'; cf. (7.8a)
N_{LSVD} cost of a left-sided singular value decomposition; cf. p. 2.21
N_{QR} cost of a QR decomposition; cf. Lemma 2.19
N_{SVD} cost of a singular value decomposition; cf. Corollary 38
$o(\cdot), O(\cdot)$ Landau symbols; cf. (4.12)
P permutation matrix (cf. (2.18)) or projection
$P_{\mathfrak{A}}$ alternator, projection onto $\mathfrak{A}(V)$; cf. (3.45)
$P_{\mathfrak{S}}$ symmetriser, projection onto $\mathfrak{S}(V)$; cf. (3.45)
$\mathbf{P}, \mathbf{P}_j$, etc. often used for projections in tensor spaces
$P_j^{\mathrm{HOSVD}}, P_{j,\mathrm{HOSVD}}^{(r_j)}, \mathbf{P}_{\mathbf{r}}^{\mathrm{HOSVD}}$ HOSVD projections; cf. Lemma 10.1

$\mathcal{P}, \mathcal{P}_p, \mathcal{P}_{\mathbf{p}}$ spaces of polynomials; cf. §10.4.2.1
Q unitary matrix of QR decomposition; cf. (2.17a)
r matrix rank or tensor rank (cf. §2.2), representation rank (cf. Definition 7.3), or bound of ranks
$\mathfrak{r}$ rank $(r_\alpha)_{\alpha\in T_D}$ connected with hierarchical format $\mathcal{H}_\mathfrak{r}$; cf. §11.2.2
r_α components of $\mathfrak{r}$ from above
$\mathbf{r}$ rank $(r_1, \ldots, r_d)$ connected with tensor subspace representation in $\mathcal{T}_\mathbf{r}$
r_j components of $\mathbf{r}$ from above
$\mathbf{r}_{\min}(\mathbf{v})$ tensor subspace rank; cf. Remark 8.4
$range(\cdot)$ range of a matrix or operator; cf. §2.1
$\mathrm{rank}(\cdot)$ rank of a matrix or tensor; cf. §2.2 and (3.24)
$\underline{\mathrm{rank}}(\cdot)$ border rank; cf. (9.11)
$\mathrm{rank}_\alpha(\cdot), \mathrm{rank}_j(\cdot)$ α-rank and j-rank; cf. Definition 5.7
$r_{\max}$ maximal rank; cf. (2.5) and §3.2.6.4
R upper triangular matrix of QR decomposition; cf. (2.17a)
$\mathbb{R}$ field of real numbers
$\mathbb{R}^J$ set of J-tuples; cf. page 4
$\mathcal{R}_r$ set of matrices or tensors of rank $\leq r$; cf. (2.6) and (3.22)
$S(\alpha)$ set of sons of a tree vertex α; cf. Definition 11.2
$\mathfrak{S}(V)$ symmetric tensor space generated by V; cf. Definition 3.62
$S(k,h)(\cdot)$ see (10.36)
$\mathrm{sinc}(\cdot)$ sinc function: $\sin(\pi x)/(\pi x)$
$\mathrm{span}\{\cdot\}$ subspace spanned by $\cdot$
$\mathrm{supp}(\cdot)$ support of a mapping; cf. §3.1.2
T_α subtree of T_D; cf. Definition 11.6
T_D dimension partition tree; cf. Definition 11.2
$T_D^{(\ell)}$ set of tree vertices at level ℓ; cf. (11.8)
T_D^{TT} linear tree used for the TT format; cf. §12
$\mathcal{T}_\mathbf{r}$ set of tensors of representation rank $\mathbf{r}$; cf. Definition 8.1
$\mathbb{T}_\rho$ set of tensors of TT representation rank $\boldsymbol{\rho}$; cf. (12.4)
$\mathrm{trace}(\cdot)$ trace of a matrix or operator; cf. (2.8) and (4.60)
$tridiag\{a,b,c\}$ tridiagonal matrix (a: lower diagonal entries, b : diagonal, c: upper diagonal entries)
U vector space, often a subspace
U, V unitary matrices of the singular value decomposition; cf. (2.19b)
u_i, v_i left and right singular vectors of SVD; cf. (2.21)
u,v,w vectors
$\mathbf{u}$,$\mathbf{v}$,$\mathbf{w}$ tensors
$\mathbf{U}$ tensor space, often a subspace of a tensor space
$\mathbf{U}_\alpha$ subspace of the tensor space $\mathbf{V}_\alpha$; cf. (11.10)
$\{\mathbf{U}_\alpha\}_{\alpha\in T_D}$ hierarchical subspace family; cf. Definition 11.8
$U', V', W', \ldots$ algebraic duals of $U, V, W, \ldots$; cf. (3.7)
$U_j^I(\mathbf{v}), U_j^{II}(\mathbf{v}), U_j^{III}(\mathbf{v}), U_j^{IV}(\mathbf{v})$ see Lemma 6.12
$U_j^{\min}(\mathbf{v}), \mathbf{U}_\alpha^{\min}(\mathbf{v})$ minimal subspaces of a tensor $\mathbf{v}$; Def. 6.3, (6.10a), and §6.4
v_i either the i-th component of v or the i-th vector of a set of vectors

$v^{(j)}$	vector of V_j corresponding to the j-th direction of the tensor; cf. §3.2.4
$\mathbf{v}^{[k]}$	tensor belonging to $\mathbf{V}_{[k]}$; cf. (3.21d)
$\mathcal{V}_{\mathrm{free}}(S)$	free vector space of a set S; cf. §3.1.2
$\mathbf{V}_\alpha$	tensor space $\bigotimes_{j\in\alpha} V_j$; cf. (5.3d)
$\mathbf{V}_{[j]}$	tensor space $\bigotimes_{k\neq j} V_j$; cf. (3.21a) and §5.2
$V, W, \ldots, X, Y, \ldots$	vector spaces
$V', W', \ldots, X', Y', \ldots$	algebraically dual vector spaces; cf. (3.7)
$\mathbf{V}, \mathbf{W}, \mathbf{X}, \mathbf{Y}$	tensor spaces
X, Y	often used for Banach spaces; cf. §4.1
$X^*, Y^*, \ldots$	dual spaces containing the continuous functionals; cf. §4.1.5
V^{**}	bidual space; cf. §4.1.5

Abbreviations and Algorithms

ALS	alternating least-squares method, cf. §9.5.2
ANOVA	analysis of variance, cf. §17.4
DCQR	cf. (2.40)
DFT	density functional theory, cf. §13.11
DFT	discrete Fourier transform, cf. §14.4.1
DMRG	density matrix renormalisation group, cf. §17.2.2
FFT	fast Fourier transform, cf. §14.4.1
HOOI	higher-order orthogonal iteration; cf. §10.3.1
HOSVD	higher-order singular value decomposition; cf. §8.3
HOSVD$(\cdot)$, **HOSVD**$^*(\cdot)$, **HOSVD**$^{**}(\cdot)$	procedures constructing the hierarchical HOSVD format; cf. (11.46a-c)
HOSVD-lw, **HOSVD*****-lw**	levelwise procedures; cf. (11.46a-c), (11.47a,b)
HOSVD-TrSeq	sequential truncation procedure; cf. (11.63)
$\mathrm{HOSVD}_\alpha(\mathbf{v})$, $\mathrm{HOSVD}_j(\mathbf{v})$	computation of HOSVD data; cf. (8.30a)
JoinBases	joining two bases; cf. (2.35)
JoinONB	joining two orthonormal bases; cf. (2.36)
LOBPCG	locally optimal block preconditioned conjugate gradient, cf. (16.13)
LSVD	left-sided reduced SVD; cf. (2.32)
MALS	modified alternating least-squares method, cf. §17.2.2
MPS	matrix product state, matrix product system; cf. §12
PEPS	projected entangled pairs states, cf. footnote 5 on page 384
PGD	proper generalised decomposition, cf. (17.1.1)
PQR	pivotised QR decomposition; cf. (2.30)
QR	QR decomposition; §2.5.2
REDUCE, **REDUCE***	truncation procedure; cf. §11.4.2
RQR	reduced QR decomposition; cf. (2.29)
RSVD	reduced SVD; cf. (2.31)
SVD	singular value decomposition; cf. §2.5.3

Part I
Algebraic Tensors

In *Chap. 1*, we start with an elementary introduction into the world of tensors (the precise definitions are in Chap. 3) and explain where large-sized tensors appear. This is followed by a description of the *Numerical Tensor Calculus*. Section 1.4 contains a preview of the material of the three parts of the book. We conclude with some historical remarks and an explanation of the notation.

The numerical tools which will be developed for tensors, make use of linear algebra methods (e.g., QR and singular value decomposition). Therefore, these matrix techniques are recalled in *Chap. 2*.

The definition of the algebraic tensor space structure is given in *Chap. 3*. This includes linear mappings and their tensor product.

Chapter 1
Introduction

In view of all that ..., the many obstacles we appear to have surmounted, what casts the pall over our victory celebration? It is the curse of dimensionality, a malediction that has plagued the scientist from earliest days.
(Bellman [11, p. 94]).

1.1 What are Tensors?

For a first rough introduction into tensors, we give a preliminary definition of tensors and the tensor product. The formal definition in the sense of multilinear algebra will be given in Chap. 3. In fact, below we consider three types of tensors which are of particular interest in later applications.

1.1.1 Tensor Product of Vectors

While vectors have entries v_i with one index and matrices have entries M_{ij} with two indices, tensors will carry d indices. The natural number[1] d defines the *order* of the tensor. The indices

$$j \in \{1, \ldots, d\}$$

correspond to the 'j-th direction', 'j-th position', 'j-th dimension', 'j-th axis', 'j-th site', or[2] 'j-th mode'. The names 'direction' and 'dimension' originate from functions $f(x_1, \ldots, x_d)$ (cf. §1.1.3), where the variable x_j corresponds to the j-th spatial direction.

For each $j \in \{1, \ldots, d\}$ we fix a (finite) index set I_j, e.g., $I_j = \{1, \ldots, n_j\}$. The Cartesian product of these index sets yields

$$\mathbf{I} := I_1 \times \ldots \times I_d \,.$$

The elements of $\mathbf{I}$ are multi-indices or d-tuples $\mathbf{i} = (i_1, \ldots, i_d)$ with $i_j \in I_j$. A tensor $\mathbf{v}$ is defined by its entries

$$\mathbf{v}_\mathbf{i} = \mathbf{v}[\mathbf{i}] = \mathbf{v}[i_1, \ldots, i_d] \in \mathbb{R}.$$

[1] The letter d is chosen because of its interpretation as spatial dimension.

[2] The usual meaning of the term 'mode' is 'eigenfunction'.

W. Hackbusch, *Tensor Spaces and Numerical Tensor Calculus*, Springer Series in Computational Mathematics 42, DOI 10.1007/978-3-642-28027-6_1,

We may write $\mathbf{v} := (\mathbf{v}[\mathbf{i}])_{\mathbf{i}\in\mathbf{I}}$. Mathematically, we can express the set of these tensors by $\mathbb{R}^{\mathbf{I}}$. Note that for any index set J, $\mathbb{R}^J$ is the vector space

$$\mathbb{R}^J = \{v = (v_i)_{i\in J} : v_i \in \mathbb{R}\}$$

of dimension $\#J$ (the sign $\#$ denotes the cardinality of a set).

Notation 1.1. Both notations, $\mathbf{v}_\mathbf{i}$ with subscript $\mathbf{i}$ and $\mathbf{v}[\mathbf{i}]$ with square brackets are used in parallel. The notation with square brackets is preferred for multiple indices and in the case of secondary subscripts: $\mathbf{v}[i_1, \ldots, i_d]$ instead of $\mathbf{v}_{i_1,\ldots,i_d}$.

There is an obvious entrywise definition of the multiplication $\lambda\mathbf{v}$ of a tensor by a real number and of the (commutative) addition $\mathbf{v}+\mathbf{w}$ of two tensors. Therefore the set of tensors has the algebraic structure of a vector space (here over the field $\mathbb{R}$). In particular in scientific fields more remote from mathematics and algebra, a tensor $\mathbf{v}[i_1, \ldots, i_d]$ is regarded as data structure and called 'd-way array'.

The relation between the vector spaces $\mathbb{R}^{I_j}$ and $\mathbb{R}^{\mathbf{I}}$ is given by the tensor product. For vectors $v^{(j)} \in \mathbb{R}^{I_j}$ $(1 \le j \le d)$ we define the *tensor product*[3,4]

$$\mathbf{v} := v^{(1)} \otimes v^{(2)} \otimes \ldots \otimes v^{(d)} = \bigotimes_{j=1}^{d} v^{(j)} \in \mathbb{R}^{\mathbf{I}}$$

via its entries

$$\mathbf{v}_\mathbf{i} = \mathbf{v}[i_1, \ldots, i_d] = v^{(1)}_{i_1} \cdot v^{(2)}_{i_2} \cdot \ldots \cdot v^{(d)}_{i_d} \qquad \text{for all } \mathbf{i} \in \mathbf{I}. \tag{1.1}$$

The tensor space is written as tensor product $\bigotimes_{j=1}^{d} \mathbb{R}^{I_j} = \mathbb{R}^{I_1} \otimes \mathbb{R}^{I_2} \otimes \ldots \otimes \mathbb{R}^{I_d}$ of the vector spaces $\mathbb{R}^{I_j}$ defined by the span

$$\bigotimes_{j=1}^{d} \mathbb{R}^{I_j} = \operatorname{span}\left\{v^{(1)} \otimes v^{(2)} \otimes \ldots \otimes v^{(d)} : v^{(j)} \in \mathbb{R}^{I_j},\ 1 \le j \le d\right\}. \tag{1.2}$$

The generating products $v^{(1)} \otimes v^{(2)} \otimes \ldots \otimes v^{(d)}$ are called *elementary tensors*.[5] Any element $\mathbf{v} \in \bigotimes_{j=1}^{d} \mathbb{R}^{I_j}$ of the tensor space is called a (general) *tensor*. It is important to notice that, in general, a tensor $\mathbf{v} \in \bigotimes_{j=1}^{d} \mathbb{R}^{I_j}$ is not representable as elementary tensor, but only as a linear combination of such products.

The definition (1.2) implies $\bigotimes_{j=1}^{d} \mathbb{R}^{I_j} \subset \mathbb{R}^{\mathbf{I}}$. Taking all linear combinations of elementary tensors defined by the unit vectors, one easily proves $\bigotimes_{j=1}^{d} \mathbb{R}^{I_j} = \mathbb{R}^{\mathbf{I}}$. In particular, because of $\#\mathbf{I} = \prod_{j=1}^{d} \#I_j$, the dimension of the tensor space is

$$\dim\left(\bigotimes_{j=1}^{d} \mathbb{R}^{I_j}\right) = \prod_{j=1}^{d} \dim(\mathbb{R}^{I_j}).$$

[3] In some publications the term '*outer product*' is used instead of 'tensor product'. This contradicts another definition of the outer product or exterior product satisfying the antisymmetric property $u \wedge v = -(v \wedge u)$ (see page 82).

[4] The index j indicating the 'direction' is written as upper index in brackets, in order to let space for further indices placed below.

[5] Also the term 'decomposable tensors' is used. Further names are 'dyads' for $d = 2$, 'triads' for $d = 3$, etc. (cf. [139, p. 3]).

Remark 1.2. Let $\#I_j = n$, i.e., $\dim(\mathbb{R}^{I_j}) = n$ for $1 \le j \le d$. Then the dimension of the tensor space is n^d. Unless both n and d are rather small numbers, n^d is a huge number. In such cases, n^d may exceed the computer memory by far. This fact indicates a practical problem, which must be overcome.

The set of matrices with indices in $I_1 \times I_2$ is denoted by $\mathbb{R}^{I_1 \times I_2}$.

Remark 1.3. (a) The particular case $d = 2$ leads to matrices $\mathbb{R}^{\mathbf{I}} = \mathbb{R}^{I_1 \times I_2}$, i.e., matrices may be identified with tensors of order 2. To be precise, the tensor entry $\mathbf{v}_{\mathbf{i}}$ with $\mathbf{i} = (i_1, i_2) \in \mathbf{I} = I_1 \times I_2$ is identified with the matrix entry M_{i_1,i_2}. Using the matrix notation, the tensor product of $v \in \mathbb{R}^{I_1}$ and $w \in \mathbb{R}^{I_2}$ equals

$$v \otimes w = v\, w^{\mathsf{T}}. \tag{1.3}$$

(b) For $d = 1$ the trivial identity $\mathbb{R}^{\mathbf{I}} = \mathbb{R}^{I_1}$ holds, i.e., vectors are tensors of order 1.

(c) For the degenerate case $d = 0$, the empty product is defined by the underlying field: $\bigotimes_{j=1}^{0} \mathbb{R}^{I_j} = \mathbb{R}$.

1.1.2 Tensor Product of Matrices, Kronecker Product

Let d pairs of vector spaces V_j and W_j $(1 \le j \le d)$ and the corresponding tensor spaces

$$\mathbf{V} = \bigotimes_{j=1}^{d} V_j \quad \text{and} \quad \mathbf{W} = \bigotimes_{j=1}^{d} W_j$$

be given together with linear mappings

$$A^{(j)} : V_j \to W_j.$$

The tensor product of the $A^{(j)}$, the so-called *Kronecker product*, is the linear mapping

$$\mathbf{A} := \bigotimes_{j=1}^{d} A^{(j)} : \mathbf{V} \to \mathbf{W} \tag{1.4a}$$

defined by

$$\bigotimes_{j=1}^{d} v^{(j)} \in \mathbf{V} \quad \mapsto \quad \mathbf{A}\left(\bigotimes_{j=1}^{d} v^{(j)}\right) = \bigotimes_{j=1}^{d} \left(A^{(j)} v^{(j)}\right) \in \mathbf{W} \tag{1.4b}$$

for[6] all $v_j \in V_j$. Since $\mathbf{V}$ is spanned by elementary tensors (cf. (1.2)), equation (1.4b) defines $\mathbf{A}$ uniquely on $\mathbf{V}$ (more details in §3.3).

[6] In De Lathauwer et al. [41, Def. 8], the matrix-vector multiplication $\mathbf{A}\mathbf{v}$ by $\mathbf{A} := \bigotimes_{j=1}^{d} A^{(j)}$ is denoted by $\mathbf{v} \times_1 A^{(1)} \times_2 A^{(2)} \cdots \times_d A^{(d)}$, where $\times_j$ is called the *j-mode product*.