SURVEY ON TENSOR BASED COMPUTATION AND MODELLING

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ABSTRACT

High-dimensional modeling is becoming ubiquitous in science and engineering due to advances in sensor technology and storage technology. The current NSF promotion of "computational thinking" is timely: we need to focus an international effort to oversee the transition from matrix-based to tensor-based computing Considerations. The tools for successful problem solving provided by the numerical linear algebra community need to be expanded and generalized. However, tensor-based research is not the only one Matrix-based research with additional subscripts. Tensors are data objects in their own right, and there is much to learn about their geometry and their connections to statistics and operator theory. NSF can help ensure the vitality of "Big N" engineering and science by systematically supporting research in tensor-based computation and modeling.

Keyword: - High-dimensional, NSF, matrix-based, tensor-based etc.

1. INTRODUCTION

A tensor is a component of the tensor product of a vector space. Up to the choice of base, it can be represented as a multidimensional array of numerical values on which algebraic operations generalizing matrix operations can be performed. In this representation, the entries in a k-th order tensor are identified by a k-tuple of subscripts, e.g., A(i1, i2, i3, i4). A matrix is a second-order tensor. A vector is a first-order tensor. A scalar is a tensor of order zero. The discretization of a continuous multivariate function on a grid yields a tensor, e.g., A(i, j, k, l) might house the value of f(w, x, y, z) at (w, x, y, z)=(wi, xj, yk, zl). In other settings, a tensor might capture an n-way interaction, e.g., A(i, j, k, l) is a value that captures an interaction between four variables/factors.

Tensors have existed since the mid-1800s and play an important role in physics, engineering, and mathematics, with varying levels of abstraction. For example, Einstein's entire theory of relativity was written in tensor form. Our use of this term will be specific and concrete: a tensor is the n-way of real (or complex) numbers. Handling such objects involves polylinear algebra. For an abstract, non-numerical treatment of that topic, see Greub [1].

1.1 Tensor-Based Computation Is Not New

Over the last four decades the fields of chemometrics and psychometrics have developed the infrastructure for tensor-based computation, see Tucker [2]. It is essential to understand this research and its intersection with numerical linear algebra. The multiway analysis texts by Smilde, Bro, and Geladi [3] and the survey article by Kolda and Bader [4] with their many references are excellent for this purpose. See also the expository papers of Bro [5] and Bro [6]. A separate literature dealing with tensor calculations has developed in the quantum chemistry and electronic structures communities. See White et al [7], Head-Gordon et al [8], Hirata [9], and Chan et al [10]. Each of these research's threads brings something unique to the table. Different camps should be intermingled so as not to reinvent the wheel.

1.2 Increasingly about big data and high dimensionality

In his acceptance speech for the Innovations Award at KDD 2007, U. Fayyad noted that Yahoo! Inc. The data retrieved by a crawl covering billions of web pages is approximately five petabytes. Another "big data" framework arises in the analysis of large social networks, where there are millions of nodes with billions of conversations. See Leskovec and Horvitz [11]. Collecting and storing large datasets of commodity, sensor data, social network data, fMRI medical data with terabyte disks is easier than ever. This data explosion creates profound research challenges that require scalable, tensor-based algorithms.

The "volume" of a tensor is the product of the component dimensions n1, n2,..., nd and therein lies the curse of dimensionality. In many applications N = n1, n2,..., nd is big primarily because d is big. And d is getting bigger because researchers are interested in developing more 2 sophisticated models that capture multiple interactions instead of idealized, overly-simplistic pairwise interactions.

The development of tensor-based methods in the numerical optimization community illustrates this point. Research in this area began with tensor methods for nonlinear equations. where the Newton iteration is extended to a low-rank approximation for the next term. In the Taylor series after the Jacobian. The technique was then extended to an optimization strategy by incorporating low-rank approximations beyond third- and fourth-order tensors Hessian matrix.

A comparative attempt has been made to "use more" terms in power series expansions for multivariate functions f(x1, x2,...,xn) in statistical settings. Truncated versions of the expansion provide a framework for modeling and computation. Generally, higher-order cumulants in the expansion are neglected, e.g., the 3rd cumulant skewness and the 4th cumulant kurtosis are both tensors. These tensors describe the higher-order dependence of random variables and can be used to estimate higher-order portfolio statistics in financial modeling situations. Just as principal components analysis (PCA) identifies factors that account for variance in covariance, principal cumulant components analysis (PCCA) identifies factors that simultaneously account for variance in all higher-order cumulants. See Morton and Lim [12]. It can be argued that the current financial crisis is partly due to the adoption of crude, tensorless, risk estimates.

1.3 Matrix to Tensor: A Complex Extrapolation

A tensor can be thought of as a higher-order matrix. Conversely, a matrix with a nested block structure can be referred to as a tensor. For example, A(1 : n1, 1 : n2, ..., 1 : n6) is an n1-by-n2 block matrix whose entries are n3-by-n4 block matrices whose entries are n5-by-n6 matrices of real numbers. Given these point-of-view alternatives, 3 the revolution of tensor-based scientific computing has ushered in a new chapter in the field of matrix calculus, not surprisingly, as the field seems to have "raised" its level of thinking. About every twenty years:

		Scalar-Level Thinking		
1960's	\Rightarrow	ψ	\$	The factorization paradigm: LU , LDL^T , QR , $U\Sigma V^T$, etc.
		Matrix-Level Thinking		
1980's	\Rightarrow	ţ	\$	Cache utilization, parallel com- puting, LAPACK, etc.
		Block Matrix-Level Thinking		
2000's	\Rightarrow	ψ	¢	New applications, factorizations, data structures, nonlinear analy-
		Tensor-Level Thinking		sis, optimization strategies, etc.

Linear algebra is a unique way to extend computational thinking from the particular to the general. The numerical PDE community led to the development of the first sparse matrix solvers in the 1950s and 1960s, a technology that now permeates science and engineering. Similar application-driven, coming-of-age stories apply to orthogonal matrix computing (statistics, 1970s), structured matrix computing (control engineering, 1980s), parallel matrix computing (real-time signal processing, 1980s), and, most recently, model-based Matrix Computation (Information Science, 2000). Tensor-based methods are under development in many application areas. It is important to identify these areas and the common ground between them from an algorithmic, analytical and software perspective.

2. CHALLENGING ALGORITHMS

2.1 Coping with the Curse of Dimensionality

There are many an approach to the curse of dimensionality involved in the manipulation of higher-order tensors. Approximation and Separability are very important. By representing functions of several variables as sums of divided functions, one gets a way to bypass the curse of dimensionality. Research in this direction should torque software development. To have multiple users of the same software on different applications, we need adaptive algorithms that guarantee accuracy and map well to some "standard" data structure. This, in turn, requires a systematic way of approximating and representing operators, particularly in mathematical physics. Tensor networks are another vehicle for representing massive vectors that arise in context Solving Hamiltonian eigenvalue problems in quantum chemistry. A tensor network is a way to represent a very high-order tensor by connecting many low-order tensors through contraction.

2.2 Numerical Linear Algebra Framework

In the field of matrix calculus Current threads of research include (a) the discovery of new computable matrix decompositions that expand the set of solvable problems, (b) the exploitation of special structures such as eccentricity and symmetry, and (c) the careful framing of numerical rank and conditioning problems by singular value decompositions. A generalization of these correlated occupations is evident at the tensor level. However, the polynomial complexity makes it clear that you can only run so far with 10 classical numerical linear algebra paradigms. For matrices, it is clear what a particular decomposition reveals. This is not always true for tensors. For matrices, our interest in data-sparse representations increases with n. For tensors, they are more likely to increase with order d and require very different strategies. For a matrix, the concept of rank is obvious for tensors it is fuzzy and ambiguous.

2.3 Decomposition Paradigm

The classical PARAFAC/CANDECOMP and Tucker tensor decompositions are discussed in Kolda and Bader (2009) together with several variants and also Comon (2001). Choosing the "right" decomposition depends on the underlying application. For example, three-way DEDICOM (decomposition into directional components) is an algebraic model similar to multidimensional scaling for the analysis of asymmetric 3-way arrays. PARAFAC2 is a modification of the popular PARAFAC (parallel component) model that is less restrictive and allows different objects in a single mode. Rather than finding a single magic decomposition, applying a range of decompositions to a given problem and drawing conclusions from the union of the insights they each provide can make "data analysis sense." In the meantime, tensor-level generalizations of the QR factorization and various eigenvalue decompositions have been explored.

2.4 Tensor Rank

In Kolda (2003), de Silva and Lim (2008), and Friedland (2008), Tensor rank is a much more difficult problem than matrix rank. This complicates the problem of computing the distance of a specified set of rank-deficient tensors for a given tensor. For example, a random 2-by-2-by-2 tensor has rank three with probability 0.79 and rank two with probability 0.21. Such a division between full rank and low rank does not occur with matriculation. For tensors the rank-related proximity question becomes ambiguous. In Ding Huang, and Luo (2008), The well-known Eckart-Young theorem can be used to express the approximation error of a matrix by their SVD. Although the exact errors cannot be expressed using the singular values of the modified/fold matrix of tensors, error bounds for tensor decompositions.

2.5 Nonnegativity

In Chicocki, Zdunek, Choi, Plemmons, Amari (2007), non-negative tensor decompositions are useful in a variety of applications ranging from document analysis to image processing to bioinformatics. They can be used for spectral unmixing for material identification with hyperspectral data and for analyzing large-scale global multivariate climate datasets. In See Kim, Sra, and Dhillon (2008), Improved Newton-type algorithms for the problem are currently being developed that overcome many computational deficiencies of existing methods.

3. CONCLUSIONS

In many respects, the "tensor" grand challenge is to solve grand challenge problems faced by data-laden researchers in other fields. Given current levels of support for information technology, biotechnology, climate modeling and other critical areas requiring sophisticated modeling and analysis of large, multidimensional datasets, funding initiatives for tensor-related research should be prioritized. By using tensors to describe mathematical objects in higher dimensions, it is clear that the development of computational polynomial algebra should parallel the development of analytical tools for higher dimensional spaces. In fact, this distinction is artificial because nonlinear approximation is the major tool that underlies both areas of research. In a very practical sense, polylinear algebra and proper approximation theory are crucial to the progress of mathematics where the curse of dimensionality is a major obstacle. The workshop highlighted the breadth of these problem areas, although there was sufficient time to focus on a subset of pertinent issues

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