Numer. Math. Theor. Meth. Appl.
doi: 10.4208/nmtma.2009.m9006s

Vol. **2**, No. 4, pp. 439-444
November 2009

Fast Revealing of Mode Ranks of Tensor in Canonical Form

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Received 15 March 2009; Accepted (in revised version) 24 June 2009

Abstract. Considering the problem of mode ranks revealing of d-dimensional array (tensor) given in canonical form, we propose fast algorithm based on cross approximation of Gram matrices of unfoldings.

AMS subject classifications: 15A21, 15A69, 19A90

Key words: Multidimensional array, canonical decomposition, Tucker approximation, fast recompression.

1. Introduction

Since d-dimensional array of size n at each dimension contains n^d elements, efficient algorithms working with multidimensional data should incorporate approximation of tensor in structured formats with much smaller number of data representation parameters. The most popular tensor formats now are canonical and Tucker. Canonical format [15] of tensor $\mathbf{F}$ with d indices $\mathbf{F} = [f_{ij\cdots k}]$ reads

$$\mathbf{F} = (A, B, \cdots, C) = \sum_{s=1}^{R} \mathbf{a}_s \otimes \mathbf{b}_s \otimes \cdots \otimes \mathbf{c}_s, \quad \text{or} \quad f_{ij\cdots k} = \sum_{s=1}^{R} a_{is} b_{js} \cdots c_{ks}, \tag{1.1}$$

where « $\otimes$ » denotes outer (Kronecker) product. Eq. (1.1) represents tensor $\mathbf{F}$ by dnR parameters and removes exponential dependence on d (so-called "curse of dimensionality"), that make canonical format very popular in computation practice, especially for large-dimensional problems. However, canonical decomposition/approximation with minimal number of summands R (referred to as *tensor rank*) is rather a complicated problem. Among several available algorithms [1–3, 6, 7, 14, 15, 18] none is known to be absolutely reliable, and many numerical packages (for example quantum chemistry package MOLPRO) compute (1.1) with very large R, what leads to excessive costs of storage and further computations.

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For more compressed data representation one can use Tucker format [21]

$$\mathbf{F} = \mathbf{G} \times_1 U \times_2 V \cdots \times_d W = \sum_{a=1}^{r_1} \sum_{b=1}^{r_2} \cdots \sum_{c=1}^{r_d} g_{ab\cdots c} \mathbf{u}_a \otimes \mathbf{v}_b \otimes \cdots \otimes \mathbf{w}_c, \qquad (1.2)$$

where coefficient tensor $\mathbf{G} = [g_{ab\cdots c}]$ is referred to as *core* and matrices $U = [\mathbf{u}_a], V = [\mathbf{v}_b], \cdots, W = [\mathbf{w}_c]$ as *mode factors.* Here « $\times_k$ » denotes multiplication of tensor by matrix along k-th mode, for example, $\mathbf{F} = \mathbf{G} \times_2 V$ means $f_{ij\cdots k} = \sum_{j'} v_{jj'} g_{ij'\cdots k}$. Summation bounds $r_1, \cdots, r_d$ are called *mode ranks* of tensor. Compression in Tucker format can be performed by reliable SVD-based algorithm [4, 5], that computes (1.2) with optimal values of mode ranks, that often turn to be considerably smaller than tensor rank and 'practical' rank R of canonical form (1.1) computed by real algorithms.

If canonical format is given for tensor $\mathbf{F}$, it can be also utilised for core $\mathbf{G}$ and total number of parameters remains linear in d. In this case it is natural to develop a method of Tucker compression, which utilises canonical structure of input. In [17] we discuss algorithm, based on low-rank approximation of canonical factors by Cross2D method. Since factors are approximated independently, total complexity is linear by d. On the other hand, accuracy criteria for approximation are estimated by inexact bounds, and this leads to overrated values for mode ranks.

In this paper we propose a new fast algorithm for mode ranks revealing and Tucker approximation of tensor in canonical form. It is based on proper decomposition of Gram matrices of unfoldings, performed by cross approximation method with linear in n complexity. Unfortunately, our method can not be applied when desired accuracy is more precise than square root of machine precision.

2. Approximation in Tucker form

Suppose $\mathbf{F}$ is given in canonical form (1.1) with large R and we need to approximate it in Tucker form (1.2) with smaller values of mode ranks $r_1, \cdots, r_d$. Standard method of Tucker approximation involves singular decompositions of all *mode unfoldings,* i.e., matrices of all mode vectors. Considering $\mathbf{F} = [f_{ij\cdots k}]$ as $n \times n^{d-1}$ matrix $F = [f_{i(j\cdots k)}]$ with row index i and column 'long index' $(j \cdots k)$, we compute SVD $F = USV^T + \Delta F$ and truncate it, introducing error $\|\Delta F\|_F \le \sqrt{d}\varepsilon \|F\|_F$. Number of dominant singular values gives mode rank r_1, and $n \times r_1$ matrix of corresponding singular vectors gives Tucker factor U. Computing factors $V, \cdots, W$ from SVD of other mode unfoldings, we write core tensor as

$$\mathbf{G} = \mathbf{F} \times_1 U^T \times_2 V^T \times_3 \cdots \times_d W^T = (U^T A, V^T B, \cdots, W^T C), \qquad (2.1)$$

preserving canonical form for core and linear number of representation parameters for $\mathbf{F}$. Accuracy of approximation is given by

$$\|\mathbf{F} - \mathbf{G} \times_1 U \times_2 V \times_3 \cdots \times_d W\|_F \le \varepsilon \|\mathbf{F}\|_F. \qquad (2.2)$$

This method is reliable, but very expensive for large-scale tensors, because SVD of $n \times n^{d-1}$ matrix requires $\mathscr{O}(n^{d+1})$ operations. Some methods with linear in n complexity are