CS 598 EVS: Tensor Computations

Course Overview

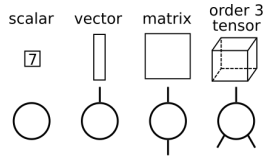
Edgar Solomonik

University of Illinois at Urbana-Champaign

Tensors

A *tensor* is a collection of elements

- its *dimensions* define the size of the collection
- its *order* is the number of different dimensions
- specifying an index along each tensor *mode* defines an element of the tensor



A few examples of tensors are

- Order 0 tensors are scalars, e.g., $s \in \mathbb{R}$
- Order 1 tensors are vectors, e.g., $\boldsymbol{v} \in \mathbb{R}^n$
- Order 2 tensors are matrices, e.g., $\boldsymbol{A} \in \mathbb{R}^{m \times n}$
- An order 3 tensor with dimensions $s_1 \times s_2 \times s_3$ is denoted as $\boldsymbol{\mathcal{T}} \in \mathbb{R}^{s_1 \times s_2 \times s_3}$ with elements t_{ijk} for $i \in \{1, \ldots, s_1\}, j \in \{1, \ldots, s_2\}, k \in \{1, \ldots, s_3\}$

Reshaping Tensors

Its often helpful to use alternative views of the same collection of elements

- *Folding* a tensor yields a higher-order tensor with the same elements
- *Unfolding* a tensor yields a lower-order tensor with the same elements
- In linear algebra, we have the unfolding $\boldsymbol{v} = \text{vec}(\boldsymbol{A})$, which stacks the columns of $\boldsymbol{A} \in \mathbb{R}^{m \times n}$ to produce $\boldsymbol{v} \in \mathbb{R}^{mn}$
- For a tensor $\boldsymbol{\mathcal{T}} \in \mathbb{R}^{s_1 \times s_2 \times s_3}$, $\boldsymbol{v} = \text{vec}(\boldsymbol{\mathcal{T}})$ gives $\boldsymbol{v} \in \mathbb{R}^{s_1 s_2 s_3}$ with

$$v_{i+(j-1)s_1+(k-1)s_1 s_2} = t_{ijk}$$

- A common set of unfoldings is given by matricizations of a tensor, e.g., for order 3,

$$\boldsymbol{T}_{(1)} \in \mathbb{R}^{s_1 \times s_2 s_3}, \boldsymbol{T}_{(2)} \in \mathbb{R}^{s_2 \times s_1 s_3}, \text{ and } \boldsymbol{T}_{(3)} \in \mathbb{R}^{s_3 \times s_1 s_2}$$

Tensor Contractions

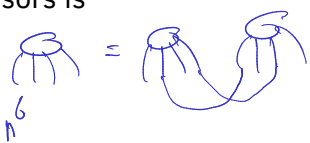
A *tensor contraction* multiplies two tensors to produce a third

- Examples: inner product, outer product, tensor product, Hadamard (elementwise) product, matrix multiplication
- One higher order example is tensor-times-matrix (TTM), e.g.,

$$t_{ijkl} = \sum_q u_{ijql} v_{qk}$$

- A common contraction between two high order tensors is

$$t_{abij} = \sum_{p,q} u_{apiq} v_{pbqj}$$



- Tensor contractions can be reduced to products of matrices and/or vectors by transposing modes and matricizing both operands, then folding and transposing the product

Tensor Contraction Expressions

In most applications, we wish to evaluate mathematical expressions involving contraction of more than two tensors

- Contractions of more than two tensors are also sometimes referred to as *einsums* (short for Einstein summation, in reference to Einstein's convention for omitting summation indices)
- One important example is the 'MTTKRP' kernel

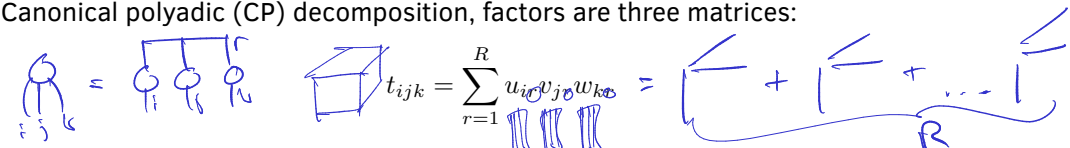
$$u_{ir} = \sum_{j,k} t_{ijk} v_{jr} w_{kr}$$

- Efficient evaluation of such kernels requires specialized algorithms
- Contraction algorithms must also be adapted to leverage tensor properties such as symmetry with respect to permutation of modes, block-wise group symmetries, and data sparsity

Tensor Decompositions

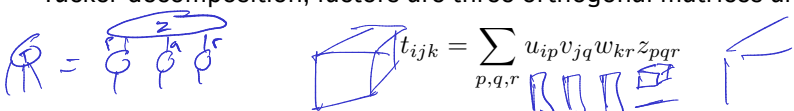
Tensor decompositions express a tensor as a contraction of *factors*

- Canonical polyadic (CP) decomposition, factors are three matrices:



$$t_{ijk} = \sum_{r=1}^{R} u_{ir} v_{jr} w_{kr}$$

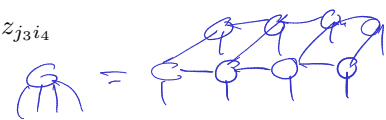
- Tucker decomposition, factors are three orthogonal matrices and a core tensor:

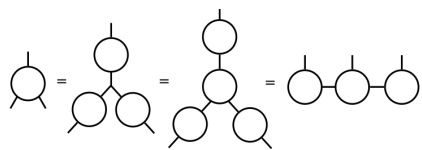


$$t_{ijk} = \sum_{p,q,r} u_{ip} v_{jq} w_{kr} z_{pqr}$$

- Tensor train decomposition, factors are matrices or order 3 tensors:

$$t_{i_1 i_2 i_3 i_4} = \sum_{j_1, j_2, j_3} u_{i_1 j_1} v_{j_1 i_2 j_2} w_{j_2 i_3 j_3} z_{j_3 i_4}$$





Applications of Tensor Decompositions

- Tensor decompositions provide a mechanism for approximating tensor datasets with a smaller number of degrees of freedom
  - polynomial improvements are obtained in electronic structure calculations
  - exponential improvements are obtained for representing some quantum states
- With imposition of constraints (e.g., nonnegativity or orthogonality), they can be used for data mining tasks such as high-order clustering
  - in the presence of missing data, tensor decompositions may be used to perform tensor completion
- When the tensor represents an operator or mapping, tensor decompositions can be used to find reduced structure
  - fast algorithms, such as FFT and Strassen's matrix multiplication algorithm, may be viewed as tensor decompositions

Tensor Decomposition Theory

- Many basic decomposition/approximation problems are formally NP-hard
- A considerable amount of theory focuses on CP decomposition and CP rank, some will be surveyed in this course
- A few alternate notions of tensor eigenvalues and singular values exist, and may be loosely tied to decompositions
- Stability and conditioning results exist for the tensor as an operator and CP decomposition as a problem

Tensor Decomposition Algorithms

- Approximation with tensor decomposition is generally formulated as a nonlinear least squares (NLS) problem
- Optimization methods usually involve successive quadratic approximation (Newton-based methods) as opposed to gradient-based methods
- Alternating least squares (ALS) decouples nonlinear problem into subproblems on subsets of variables that are quadratic and solves each in an alternating manner
- Other optimization methods, such as interior point and ADMM, are often employed in the presence of constraints
- In all cases, methods are specialized to work efficiently for tensor decompositions and may be adapted for sparsity

Tensor Networks

- Tensor network methods take as input a tensor that is already decomposed
- Goal is generally to learn something about an operator described by a tensor network
- Often want to compute extremal eigenpairs of matrix $\boldsymbol{M}$ a tensor folding of which $\boldsymbol{\mathcal{T}}$ is described by the tensor network, e.g.,

$$\boldsymbol{M} = \boldsymbol{A} \otimes \boldsymbol{B} + \boldsymbol{C} \otimes \boldsymbol{D}$$

- Unknowns, e.g., eigenvectors in eigenproblem above, often also represented implicitly by a tensor decomposition
- These methods are prevalent for studying quantum systems, which involve a Hamiltonian acting on a space that is exponential in size relative to the system
- In this context, tensor networks are also effective for time-evolution

Tensor Network Theory and Algorithms

- Different classes of functions have low rank with respect to different tensor networks
- 1D and 2D tensor networks are most widely used for quantum systems
- Successive (alternating) quadratic optimization also widely used for tensor networks
- *Canonical forms* propagate orthogonality conditions to ensure stability
- Naive contraction of 2D tensor networks has exponential cost, various approximate algorithms exist
- Other tensor networks trade-off connectivity and contractibility