## Towards efficient algorithms and systems for tensor decompositions and tensor networks

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Final exam
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## Presentation overview

Thesis motivation: design and automate fast numerical algorithms for tensor computations in science and engineering

Outline of the presentation:

- Introduction to tensors
- An overview of thesis contributions
- Sketching for tensor decompositions and tensor networks
- Algorithms for approximate tensor network contractions


## Tensor

Tensor: multi-dimensional array of data

- Order: number of dimensions of a tensor
- Dimension size: number of elements in each dimension

| vector | matrix | third order tensor |
| :---: | :---: | :---: |
| $\left[\begin{array}{l} 4 \\ 5 \end{array}\right]$ | $\left[\begin{array}{ll}1 & 2 \\ 3 & 4\end{array}\right]$ |  |

Tensors occur in

- Data science: image, video, medical data...
- Scientific computing: discretization of high-dimensional functions
- Quantum physics and quantum computing: wavefunction, Hamiltonian, quantum gate


## Tensor diagram notation

Tensor diagram: an order $N$ tensor is represented by a vertex with $N$ adjacent edges

## Scalar Vector Matrix <br> Order 3 <br> tensor <br>  <br> 

Matricization: transform a tensor into a matrix




\[

\]

$k\left[\begin{array}{llll}1 & 3 & 2 & 4 \\ 5 & 7 & 6 & 8\end{array}\right]$

## Tensor contraction

Tensor contraction: summing element products from two tensors over contracted dimensions
A dimension (edge) is contracted if it has no open end
Examples:

## (a) ${ }^{i}$ (b)

Inner product: $\sum_{i} a_{i} b_{i} \quad$ Matrix product : $C_{i k}=\sum_{j} A_{i j} B_{j k}$


Tensor times matrix: $C_{i l k}=\sum_{j} A_{i l j} B_{j k}$


Kronecker/outer product: $T_{i j k l}=A_{i k} B_{j l}$


Khatri-Rao product: $T_{i j l}=A_{i l} B_{j l}$

## Tensor decomposition: break the curse of dimensionality

Matrix factorization:


Tensor decomposition: represents a tensor with a (low-rank) tensor network

$\xrightarrow{\text { decompose }}$

Tucker decomposition



Tensor train decomposition


## Applications of tensor decompositions and tensor networks

## Tensor decompositions:

Data science: detect latent structure ${ }^{1,2}$
Quantum chemistry: accelerate high-accuracy methods ${ }^{3}$

Quantum physics: represent wavefunctions and Hamiltonians ${ }^{4}$

Tensor network contractions:
Quantum computing: simulate quantum algorithm ${ }^{5}$

[^0]
## (Rank-constrained) linear least squares with tensor networks

$$
\min _{X, \operatorname{rank}(X) \leq R}\|L X-Y\|_{F}
$$

Tucker decomposition

CP decomposition



Tensor network contraction


## An overview of thesis contributions

Accelerating alternating minimization of tensor decompositions ${ }^{1,2,3}$

- Pairwise perturbation for CP and Tucker decompositions
- AutoHOOT: an automatic differentiation system for tensors

Sketching for tensor decompositions and tensor networks ${ }^{4,5}$
Approximate tensor network contraction algorithms ${ }^{6,7}$
Use low-rank CP decomposition to simulate and analyze quantum algorithms ${ }^{8,9}$

- We simulate Grover's search, quantum Fourier transform, quantum phase estimation
- A new upper bound on CP rank of specific quantum states

[^1]
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## Sketching for linear least squares

Sketching: randomly project a data $L$ to low dimensional spaces


- $L \in \mathbb{R}^{s \times n}, S \in \mathbb{R}^{m \times s}$ with the sketch size $m \ll s$
- $S$ is a random matrix (called embedding)


## Sketching for linear least squares

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## Standard LLS:

$$
X^{*}=\underset{X}{\operatorname{argmin}}\|L X-Y\|_{F} \quad \hat{X}=\underset{X}{\operatorname{argmin}}\|S L X-S Y\|_{F}
$$

## Sketched LLS:

- Gaussian random matrix is standard for embedding
- Sparse embedding ${ }^{1}$ can be used when $L, Y$ are sparse (computing $S L$ only costs nnz( $L$ ))

[^2]
## Sketching general tensor networks

Problem: Find a tensor network embedding $S$ for the tensor network $X$, so that

- The embedding is $(\epsilon, \delta)$-accurate
- The sketch size (number of rows of $S$ ) is low
- Asymptotic cost to compute $S X$ is minimized


An (oblivious) embedding $S \in \mathbb{R}^{m \times s}$ is $(\epsilon, \delta)$-accurate if ${ }^{1}$

$$
\operatorname{Pr}\left[\left|\frac{\|S x\|_{2}-\|x\|_{2}}{\|x\|_{2}}\right|>\epsilon\right] \leq \delta \quad \text { for any } x \in \mathbb{R}^{s}
$$

[^3]
## Outline: sketching for tensor networks

$$
\min _{X}\|L X-Y\|_{F} \quad \rightarrow \quad \min _{X}\|S L X-S Y\|_{F}
$$

Sketching for low-rank Tucker decomposition of large and sparse tensors ${ }^{1}$

- $L$ is a Kronecker product of matrices and has orthonormal columns
- A new sketch size upper bound on the problem
- Reach at least $98 \%$ of the standard algorithm's accuracy with better cost

[^4]
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A cost-efficient algorithm to sketch arbitrary tensor network ${ }^{2}$

- L has arbitrary tensor network structure
- Find accurate and cost-optimal embeddings $S$
- Asymptotically faster than previous works for CP decomposition

[^5]
## Sketching for Tucker decomposition

Goal: efficiently sketch the rand-constrained linear least squares problem arising in alternating least squares for Tucker decomposition

## Alternating least squares for Tucker decomposition

Tucker decomposition

$$
\min _{G, A, B, C} \sum_{i, j, k}\left(T_{i j k}-\sum_{a, b, c} G_{a b c} A_{i a} B_{j b} C_{k c}\right)^{2}
$$

- $T \in \mathbb{R}^{s \times s \times s}, X \in \mathbb{R}^{R \times R \times R}$
- $A, B, C \in \mathbb{R}^{s \times R}$ with orthonormal columns, $R<s$


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Higher order orthogonal iteration $(\mathrm{HOOI})^{1}$

$$
\min _{X, \operatorname{rank}(X) \leq R}\|L \quad X-Y\|_{F}
$$

- Costs $\Omega(\mathrm{nnz}(T) R)$ for arbitrary tensor order
- Fast convergence (usually in around 10 iterations)


[^6]
## Sketching for Tucker decomposition: previous work

Sketch alternating unconstrained least squares (AULS) ${ }^{1}$

- Advantage: cost with $t$ iterations is $O\left(\mathrm{nnz}(T)+t\left(s R^{5}+R^{7}\right)\right)$
- Disadvantage: not an orthogonal iteration and has slow convergence


Apply sketching on high-order SVD²

- Apply randomized SVD on matricizations of $T$
- Disadvantages: accuracy lower than HOOI and costs $\Omega(\mathrm{nnz}(T) R)$

[^7]
## Sketched HOOI for Tucker decomposition

$$
\min _{X, \operatorname{rank}(X) \leq R}\|L \quad X-Y\|_{F}
$$



HOOI: solve and truncate

$$
X^{*} \leftarrow \underset{X}{\operatorname{argmin}}\|L X-Y\|_{F}^{2}
$$

$X_{R}^{*} \leftarrow$ rank- $R$ approximation of $X^{*}$

$$
G A \leftarrow X_{R}^{*}
$$

Sketched HOOI: sketch, solve and truncate

$$
\hat{X} \leftarrow \underset{X}{\operatorname{argmin}}\|S L X-S Y\|_{F}^{2}
$$

$\hat{X}_{R} \leftarrow$ rank- $R$ approximation of $\hat{X}$

$$
\hat{G} \hat{A} \leftarrow \hat{X}_{R}
$$

## Sketched HOOI for Tucker decomposition

We use efficient embeddings $S$ for solving $\min _{X}\|S L X-S Y\|_{F}^{2}$

- $L$ is a Kronecker product of factor matrices and changes over iterations
- $Y$ is a matricization of the input tensor and can be sparse

Leverage score sampling

- Sample each row of $L$ based on the leverage score vector $\ell(L)$

Tensorsketch: tensorized Countsketch ${ }^{1}$
-(5)- Countsketch matrix
-(IV- DFT matrix


[^8]
## Sketched HOOI for Tucker decomposition

We derive sketch size bounds so that

$$
\left\|L \hat{X}_{R}-Y\right\|_{F}^{2} \leq(1+O(\epsilon))\left\|L X_{R}^{*}-Y\right\|_{F}^{2}
$$

- $X_{R}^{*}, \hat{X}_{R}$ : optimal and the sketched solution
- We apply Mirsky's inequality ${ }^{1}$ to bound change in singular values of the sketched $L$
- Sketch size upper bound is at most $O(1 / \epsilon)$ times that for unconstrained LS

[^9]
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Algorithm performs well in experiments

- Sketched HOOI converges to at least $98 \%$ of the accuracy of standard HOOI
- With leverage score sampling, cost with $t$ iterations is $O\left(\mathrm{nnz}(T)+t\left(s R^{3}+R^{6}\right)\right)$

[^10]
## Sketching general tensor networks

Goal: accurately and efficiently sketch arbitrary tensor network structure

## Sketching general tensor networks

Previous work:

- Kronecker product embedding ${ }^{1}$ : inefficient in computational cost
- Tree embedding (e.g. tensor train) ${ }^{1,2}$ : efficient for specific data (Kronecker product, tensor train), but efficiency unclear for general tensor network data

[^11]
## Sketching general tensor networks

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Assumptions throughout our analysis:

- Multiply $A, B \in \mathbb{R}^{n \times n}$ has a cost of $O\left(n^{3}\right)$
- $S$ is a Gaussian tensor network defined on graphs
- Each dimension to be sketched has large size


[^12]
## Sufficient condition for $(\epsilon, \delta)$-accurate embedding

The embedding is accurate if we can rewrite $S=S_{1} \cdots S_{N}$ and

- $S_{i}$ is the Kronecker product of $A_{i}$ (a Gaussian random matrix) and identity matrices
- $A_{i}$ has row size $\Omega\left(N \log (1 / \delta) / \epsilon^{2}\right)$



## Sufficient condition for $(\epsilon, \delta)$-accurate embedding

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- $A_{i}$ has row size $\Omega\left(N \log (1 / \delta) / \epsilon^{2}\right)$


Two key prior results used in the proof ${ }^{1}$

- If $A_{i}$ is $(\epsilon, \delta)$-accurate, so is the Kronecker product between $A_{i}$ and identity matrices
- If $S_{1}, \ldots, S_{N}$ are $(\epsilon / \sqrt{N}, \delta)$-accurate, $S_{1} \cdots S_{N}$ is $(O(\epsilon), \delta)$-accurate

[^13]
## A sketching algorithm with efficient computational cost and sketch size

Embedding containing a Kronecker product embedding + bi-
 nary tree of gadgets

Each small gadget sketches the product of two tensors

- Each gadget contains a pair of tensors
- Dimension sizes in each gadget are chosen based on data tensors to minimize cost
- Can reduce cost by $O(\sqrt{m})$ compared to containing one tensor


## Analysis of the algorithm

c: asymptotic sketching cost for our algorithm
$c_{\text {opt }}$ : optimal asymptotic sketching cost under the embedding sufficient condition $m$ : sketch size

| Input data tensor network structure | Optimality of the algorithm |
| :--- | :--- |
| General hypergraph | $c=O\left(\sqrt{m} \cdot c_{\mathrm{opt}}\right)$ |
| General graph | $c=O\left(m^{0.375} \cdot c_{\mathrm{opt}}\right)$ |
| Each data tensor has a dimension to be sketched <br> (e.g. Kronecker product, tensor train) | $c=c_{\mathrm{opt}}$ |

## Applications

Low-rank CP decomposition with alternating least squares

- R: CP rank, $N$ : tensor order
- Our algorithm is $\Omega(N R)$ times better than prior work ${ }^{1}$
- Larger preparation cost is needed (can be reduced by using sparse embeddings)

Truncation of high-rank tensor train

- Our algorithm is more efficient the standard algorithm
- We show the recently proposed truncation algorithm is also optimal ${ }^{2}$

[^14]
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## Tensor network contraction

Tensor network: denoted by undirected hypergraph $G=(V, E)$
Contraction tree: rooted binary tree $T$

- A leaf of $T$ represents a tensor in $G$
- A non-leaf vertex represents its children's contraction output


Find contraction cost-optimal contraction tree: NP-hard ${ }^{1}$, many heuristics are used ${ }^{2,3}$
Cost under optimal contraction tree: exponential to the treewidth of $G$ 's line graph ${ }^{4}$

[^15]
## Approximate tensor network contractions: previous work

Idea: approximate each contraction output as a bounded-rank tensor network



Tensor train/matrix product state (MPS) ${ }^{1,2}$ Binary tree tensor network ${ }^{3}$


We propose an algorithm for cost-efficient con- We propose to contract with flexible and costtraction tree efficient low-rank approximation

[^16]
## Outline: approximate tensor network contraction algorithms

Cost-efficient contraction tree for the tensor train-based algorithm ${ }^{1}$

- Solves a linear ordering problem to minimize edge crossings
- Achieves 5.9X speed-up when compared to previous works

Contraction with a flexible and cost-efficient low-rank approximation ${ }^{2}$

- Uses normal equations to improve efficiency and can flexibly select the environment
- Achieves 9.2X speed-up when compared to previous works

[^17]
## Accelerate tensor train-based algorithm

Goal: find efficient contraction trees for tensor train-based approximate tensor network contraction

## Contraction of two tensor trains into a tensor train

Algorithm: move contracted edges to the center through adjacent swaps, then eliminate them ${ }^{1}$

- Each swap uses low-rank approximation to maintain a bounded rank


Observation: The total number of swaps is lower bounded by the convex crossing number ${ }^{2}$

[^18]
## CATN-GO: build contraction tree constrained by a vertex ordering

Our approach: find a vertex ordering that minimizes edge crossings, then find a contraction tree constrained by the ordering

- Inspired by prior work on building exact tensor network contraction trees ${ }^{1}$



Find the optimal vertex ordering: NP-hard problem, heuristics are used ${ }^{2}$

Contraction tree optimization: minimize the cost using dynamic programming

[^19]
## Experimental results



Results for contracting an Ising model tensor network defined on a $5 \times 5 \times 5$ lattice

- Number on each point: maximum tensor train rank
- Achieve 5.9X speed-up relative to previous works to reach a relative error of $10^{-8}$

[^20]
## Efficient low-rank approximation for tensor network contraction

Goal: efficiently and accurately perform low-rank approximation in approximate tensor network contraction

## Motivation for a new low-rank approximation subroutine

$$
\min _{X, \operatorname{rank}(X) \leq R}\|L X-L B\|_{F}
$$



Accuracy: environment $(L)$ typically comprises a small part of the whole tensor network ${ }^{1,2}$

- Small $L \rightarrow$ minimizes local rather than global error

Efficiency: Orthogonalization (via implicit QR factorization) on $L$ is performed

- QR factorization can be expensive when $L$ is not a tree

[^21]
## Normal equations for low-rank approximation

$$
X^{*}=\underset{X, \operatorname{rank}(X) \leq r}{\operatorname{argmin}}\|L X-L B\|_{F}
$$

Orthogonalization-based: $Q_{L}, R_{L} \leftarrow \mathrm{QR}(L)$, then use the rank- $r$ approximation of $R_{L} B$ to update solution

Normal equations-based: compute the leading $r$ eigenvectors of $B^{T} L^{\top} L B$, and $X^{*}=B V V^{\top}$

The asymptotic cost to form normal equations $\left(B^{T} L^{T} L B\right)$ is upper-bounded by doing QR

## Partitioned Contract: use partial contraction tree for flexible environment

Contraction tree over partitions
Complete contraction tree


Each contraction outputs a binary tree tensor network

- The input pair of partitions are considered the environment
- Larger partition implies larger environment $\rightarrow$ minimizes the global error


## Experimental results



Results for contracting an Ising model tensor network defined on a $5 \times 5 \times 5$ lattice

- Number on each point: maximum tensor train rank
- Achieve 9.2X speed-up relative to previous works to reach a relative error of $10^{-9}$

[^22]
## Conclusion

Introduce efficient numerical algorithms for tensor decompositions and tensor networks

Applications include machine learning with large-scale datasets and simulation of large quantum circuits

Our contributions to tensor network libraries automate the development of fast algorithms

## Future work

Tensor network sketching

- Generalize the analysis to other embeddings, such as Countsketch ${ }^{1}$ and Tensorsketch ${ }^{2}$

Approximate tensor network contraction

- For CATN-GO: devise heuristics for finding vertex orderings with fewer edge crossings
- For Partitioned Contract: find efficient partial contraction trees

[^23]
## Backup slides

## Experimental results

| Vertex ordering | $8 \times 8 \times 8$ lattice |  |  | $(6,300)$-rand regular graph |  |  |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
|  | \# crossings | Time (s) | GFlops | \# crossings | Time (s) | GFlops |
| Baseline | 34.6 k | 2.2 k | 9.4 k | 133 k | 10.8 k | 52 k |
| Recursive bisection | 16.8 k | 1.0 k | 4.6 k | 37.5 k | 2.8 k | 13.8 k |
| Relative improvements | 2.1 X | 2.2 X | 2.1 X | 3.5 X | 3.8 X | 3.8 X |

Vertex orderings with fewer edge crossings yield less contraction time

- Baseline: sequential traversal for lattice, and random ordering for a random graph
- Random regular graph has 300 vertices and degree 6


## Analysis of the sketching algorithm

Lower bound analysis

- When the data contains 2 tensors, sketching lower bound can be derived
- Kronecker product case: when the data has two vectors with size $m$ (sketch size), the sketching computational cost is $\Omega\left(m^{2.5}\right)$
- When the data has more tensors, for a given contraction path the lower bound is the sum of two-tensor-contraction lower bounds
Algorithm design
- For the 2-tensor data, can design embedding attaining the lower bound

- For the data with more tensors, we can derive the optimal way to sketch using the two-tensor scheme for a given contraction path
- We can try all data contraction paths to get the optimal sketching path


## Example: sketching Kronecker product data

Consider contracting an input Kronecker product from left to the right

Sketching contraction path as follows


Our algorithm reduces cost by up to $O(\sqrt{m})$ for the same accuracy compared to using tree embeddings ${ }^{1}$

[^24]
## Randomized SVD using sketching

Given a matrix $A \in \mathbb{R}^{m \times n}$, find a rank- $r$ approximation with $r \ll m, n$ in the SVD form
Randomized range finder ${ }^{1}$

- Generate a random embedding matrix $\Omega \in \mathbb{R}^{n \times \Theta(r)}$

- $Q, R \leftarrow \operatorname{qr}(A \Omega)$, so $Q \in \mathbb{R}^{m \times \Theta(r)}$

Dimensionality reduction

- $B \leftarrow Q^{T} A$


SVD on the low-rank matrix $Q B$

- $Q_{B}, \Sigma, V_{B}^{T} \leftarrow \operatorname{svd}(B)$
- Return $Q Q_{B}, \Sigma, V_{B}^{T}$


[^25]
## Experiments: sketching a MPS data




- Input MPS: order 6, each dimension size $s=500$ with varying MPS rank
- TN embedding: Kronecker product + a binary tree of small networks
- Tree embedding: Kronecker product + a binary tree tensor network
- Sketching error is within 0.1
- Our TN embedding achieves the best asymptotic cost for all MPS ranks


## Experiments: sketching a Kronecker product data




- Input data: each dimension size $s=1000$ with varying number of orders
- Sketching error is within 0.1
- Our TN embedding achieves the best asymptotic cost
- TN, tree, and MPS embeddings have efficient sketch size


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