Towards efficient algorithms and systems for tensor decompositions and tensor networks

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Final exam

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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		
$\begin{bmatrix} 4 \\ 5 \end{bmatrix}$	$\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}$	$\begin{bmatrix}1\begin{bmatrix}5\\7\\3\end{bmatrix}^{6}\\8\end{bmatrix}$		

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

Matricization: transform a tensor into a matrix





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:

 $i \stackrel{i}{\bigoplus} i \stackrel{j}{\bigoplus} k \qquad i \stackrel{j}{\bigoplus} k$ Inner product: $\sum_{i} a_{i}b_{i}$ Matrix product : $C_{ik} = \sum_{j} A_{ij}B_{jk}$ Tensor times matrix: $C_{ilk} = \sum_{j} A_{ilj}B_{jk}$ $i \stackrel{i}{\longrightarrow} k \qquad \qquad i \stackrel{i}{\longrightarrow} l$ Kronecker/outer product: $T_{ijkl} = A_{ik}B_{jl}$ Khatri-Rao product: $T_{ijl} = A_{il}B_{jl}$

Tensor decomposition: break the curse of dimensionality

Matrix factorization:

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



Applications of tensor decompositions and tensor networks

Tensor decompositions:

Data science: detect latent structure^{1,2}

 $\label{eq:Quantum chemistry: accelerate high-accuracy methods^3$

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

Tensor network contractions:

 $\label{eq:Quantum computing: simulate quantum algorithm^{5}$



 $^{^1{\}rm Kolda}$ and Bader, Tensor decompositions and applications, SIAM review 2009

²Sidiropoulos et al, Tensor decomposition for signal processing and machine learning, IEEE Signal Processing 2017

³Hohenstein et al, Communication: Tensor hypercontraction. III. Least-squares tensor hypercontraction for the determination of correlated wavefunctions, JCS 2012

⁴Verstraete et at, Matrix product states, projected entangled pair states, and variational renormalization group methods for quantum spin systems, Advances in physics 2008

⁵Markov and Shi, Simulating quantum computation by contracting tensor networks, SIAM Journal on Computing 2008

(Rank-constrained) linear least squares with tensor networks

 $\min_{X,\mathrm{rank}(X)\leq R} \ ig| \ L \ X \ - \ Y \ ig|_F$



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[Ma and Solomonik, NLA 2022] ²[Ma and Solomonik, IPDPS 2021] ³[Ma, Ye and Solomonik, PACT 2020] ⁴[Ma and Solomonik, NeurIPS 2021] ⁵[Ma and Solomonik, NeurIPS 2022] ⁶[Ma, Ibrahim, Safro, and Solomonik, in preparation] ⁷[Ma, Fishman, Stoudenmire, and Solomonik, in preparation] ⁸[Ma and Yang, JCS 2022] ⁹[Schatzki, Ma, Solomonik, and Chitambar, 2022]

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Sketching for linear least squares

Sketching: randomly project a data L to low dimensional spaces

 $L \longrightarrow SL$

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

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Standard LLS: Sketched LLS:

$$X^* = \underset{X}{\operatorname{argmin}} \|LX - Y\|_F \qquad \qquad \hat{X} = \underset{X}{\operatorname{argmin}} \|SLX - SY\|_F$$

- Gaussian random matrix is standard for embedding
- Sparse embedding¹ can be used when L, Y are sparse (computing SL only costs nnz(L))

¹Charikar et al, Finding frequent items in data streams, 2002

Sketching general tensor networks

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

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



An (oblivious) embedding $S \in \mathbb{R}^{m \times s}$ is (ϵ, δ) -accurate if¹

$$\Pr\left[\left|\frac{\|Sx\|_2 - \|x\|_2}{\|x\|_2}\right| > \epsilon\right] \le \delta \quad \text{for any } x \in \mathbb{R}^s$$

 $^1 {\rm Woodruff}, \, {\rm Sketching} \mbox{ as a tool for numerical linear algebra, 2014}$

Outline: sketching for tensor networks

$$\min_{X} \|LX - Y\|_{F} \quad \rightarrow \quad \min_{X} \|SLX - SY\|_{F}$$

Sketching for low-rank Tucker decomposition of large and sparse tensors¹

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

 $^{^1}$ Ma and Solomonik, Fast and accurate randomized algorithms for low-rank tensor decompositions, NeurIPS 2021

Outline: sketching for tensor networks

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Sketching for low-rank Tucker decomposition of large and sparse tensors¹

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A cost-efficient algorithm to sketch arbitrary tensor network²

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

 $^{^{1}}$ Ma and Solomonik, Fast and accurate randomized algorithms for low-rank tensor decompositions, NeurIPS 2021 2 Ma and Solomonik, Cost-efficient Gaussian tensor network embeddings for tensor-structured inputs, NeurIPS 2022

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

$$\min_{G,A,B,C}\sum_{i,j,k}\left(T_{ijk}-\sum_{a,b,c}G_{abc}A_{ia}B_{jb}C_{kc}\right)^{2}$$

•
$$T \in \mathbb{R}^{s imes s imes s}$$
, $X \in \mathbb{R}^{R imes R imes R}$

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



Alternating least squares for Tucker decomposition

Tucker decomposition

$$\min_{G,A,B,C}\sum_{i,j,k}\left(T_{ijk}-\sum_{a,b,c}G_{abc}A_{ia}B_{jb}C_{kc}\right)^{2}$$

•
$$\mathcal{T} \in \mathbb{R}^{s imes s imes s}$$
, $X \in \mathbb{R}^{R imes R imes R}$

• $A, B, C \in \mathbb{R}^{s imes R}$ with orthonormal columns, R < s

Higher order orthogonal iteration (HOOI)¹

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



$$\lim_{X, \operatorname{rank}(X) \leq R} || L X = 1 || F$$

$$j = 0$$

$$k = 0$$

$$k = 0$$

$$k = 1$$

min

¹Lathauwer et al, On the best rank-1 and rank- (R_1, R_2, \ldots, R_n) approximation of higher-order tensors, SIMAX 2000

Sketching for Tucker decomposition: previous work

Sketch alternating unconstrained least squares (AULS)¹

- Advantage: cost with t iterations is $O(nnz(T) + t(sR^5 + R^7))$
- Disadvantage: not an orthogonal iteration and has slow convergence



Apply sketching on high-order SVD^2

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

 $^{^1}$ Malik and Becker, Low-rank tucker decomposition of large tensors using Tensorsketch, NeurIPS 2018 2 Ahmadi-Asl et al, Randomized algorithms for computation of Tucker decomposition and HOSVD, IEEE Access 2021

$$\min_{X,\mathrm{rank}(X)\leq R} \left| \left| \begin{array}{ccc} L & X & - \end{array} \right. Y \left| \left|_F \right.
ight|
ight|_F$$



HOOI: solve and truncate

Sketched HOOI: sketch, solve and truncate

$$X^* \leftarrow \operatorname*{argmin}_X \| LX - Y \|_F^2$$

 $X_R^* \leftarrow \text{rank-}R \text{ approximation of } X^*$ $GA \leftarrow X_R^*$

 $\hat{X} \leftarrow \operatorname{argmin} \|SLX - SY\|_{F}^{2}$

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

 $\hat{G}\hat{A} \leftarrow \hat{X}_R$

We use efficient embeddings S for solving $\min_X ||SLX - SY||_F^2$

- 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 Countsketch¹







 1 Pham and Pagh, Fast and scalable polynomial kernels via explicit feature maps, KDD 2013

Efficient algorithms for tensors

We derive sketch size bounds so that

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

- X_R^*, \hat{X}_R : optimal and the sketched solution
- We apply Mirsky's inequality¹ 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

¹Mirsky, The Quarterly journal of mathematics, 1960

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Algorithm performs well in experiments

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

¹Mirsky, The Quarterly journal of mathematics, 1960

Goal: accurately and efficiently sketch arbitrary tensor network structure

Sketching general tensor networks

Previous work:

- Kronecker product embedding¹: 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

 $^{^1 \}rm Ahle$ et al, Oblivious sketching of high-degree polynomial kernels, SODA 2020 $^2 \rm Rakhshan$ and Rabusseau, Tensorized random projections, AISTATS 2020

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Assumptions throughout our analysis:

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



¹Ahle et al, Oblivious sketching of high-degree polynomial kernels, SODA 2020 ²Rakhshan and Rabusseau, Tensorized random projections, AISTATS 2020

Sufficient condition for (ϵ, δ) -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 $\Omega(N \log(1/\delta)/\epsilon^2)$



Sufficient condition for (ϵ, δ) -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 $\Omega(N \log(1/\delta)/\epsilon^2)$



Two key prior results used in the proof¹

- If A_i is (ϵ, δ) -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

¹Ahle et al, Oblivious sketching of high-degree polynomial kernels, SODA 2020

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Efficient algorithms for tensors

A sketching algorithm with efficient computational cost and sketch size



Embedding containing a Kronecker product embedding + binary 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_{opt} : optimal asymptotic sketching cost under the embedding sufficient condition m: sketch size

Input data tensor network structure	Optimality of the algorithm		
General hypergraph	$c = O(\sqrt{m} \cdot c_{ ext{opt}})$		
General graph	$c = O(m^{0.375} \cdot c_{opt})$		
Each data tensor has a dimension to be sketched (e.g. Kronecker product, tensor train)	$c = c_{\rm opt}$		

Applications

Low-rank CP decomposition with alternating least squares

- R: CP rank, N: tensor order
- Our algorithm is $\Omega(NR)$ times better than prior work¹
- 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
- \bullet We show the recently proposed truncation algorithm is also $\mathsf{optimal}^2$

 $^{^1}$ Malik, More Efficient Sampling for Tensor Decomposition With Worst-Case Guarantees, ICML 2022 2 Daas et al, Randomized algorithms for rounding in the Tensor-Train format, SISC 2023

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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-hard¹, many heuristics are used^{2,3}

Cost under optimal contraction tree: exponential to the treewidth of G's line graph⁴

¹O'Gorman, Parameterization of Tensor Network Contraction, TQC 2019

²Gray and Kourtis, Hyper-optimized tensor network contraction, Quantum 2021

³Liu et al, Computing solution space properties of combinatorial optimization problems via generic tensor networks, SISC 2023

⁴Markov and Shi, Simulating quantum computation by contracting tensor networks, SIAM Journal on Computing 2008

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 network³

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

¹Pan et al, Contracting arbitrary tensor networks: general approximate algorithm and applications in graphical models and quantum circuit simulations, PRL 2020

³ Jermyn, Automatic contraction of unstructured tensor networks, SciPost Physics 2020

²Chubb, General tensor network decoding of 2D Pauli codes, 2021

Outline: approximate tensor network contraction algorithms

Cost-efficient contraction tree for the tensor train-based algorithm¹

- 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 approximation²

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

 $^{{}^{1}}Ma$, Ibrahim, Safro, and Solomonik, An efficient swap-based algorithm for approximate tensor network contractions, in preparation

 $^{^{2}}$ Ma, Fishman, Stoudenmire, and Solomonik, Tensor network contraction with flexible environment incorporation and a cost-efficient density matrix algorithm for tree approximation, in preparation

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 them¹

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



Observation: The total number of swaps is lower bounded by the convex crossing number²

²Shahrokhi et al, Book embeddings and crossing numbers, WG'94

¹Pan et al, Contracting arbitrary tensor networks: general approximate algorithm and applications in graphical models and quantum circuit simulations, PRL 2020

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 trees¹



Find the optimal vertex ordering: NP-hard problem, heuristics are used²

Contraction tree optimization: minimize the cost using dynamic programming

¹Ibrahim et al, Constructing Optimal Contraction Trees for Tensor Network Quantum Circuit Simulation, HPEC 2022 ²Shahrokhi et al, Book embeddings and crossing numbers, WG'94

Experimental results



Results for contracting an Ising model tensor network defined on a $5\times5\times5$ lattice

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

¹Chubb, General tensor network decoding of 2D Pauli codes, 2021

²Pan et al, Contracting arbitrary tensor networks: general approximate algorithm and applications in graphical models and quantum circuit simulations, PRL 2020

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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



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

²Chubb, General tensor network decoding of 2D Pauli codes, 2021

¹Pan et al, Contracting arbitrary tensor networks: general approximate algorithm and applications in graphical models and quantum circuit simulations, PRL 2020

Normal equations for low-rank approximation

$$X^* = \operatorname*{argmin}_{X, \mathsf{rank}(X) \leq r} \|LX - LB\|_F$$

Orthogonalization-based: $Q_L, R_L \leftarrow QR(L)$, then use the rank-*r* approximation of $R_L B$ to update solution

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

The asymptotic cost to form normal equations $(B^T L^T L B)$ 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
- \bullet Larger partition implies larger environment \rightarrow minimizes the global error

Experimental results



Results for contracting an Ising model tensor network defined on a $5\times5\times5$ lattice

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

²Chubb, General tensor network decoding of 2D Pauli codes, 2021

¹Pan et al, Contracting arbitrary tensor networks: general approximate algorithm and applications in graphical models and quantum circuit simulations, PRL 2020

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

Tensor network sketching

• Generalize the analysis to other embeddings, such as Countsketch¹ and Tensorsketch²

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

²Pham and Pagh, Fast and scalable polynomial kernels via explicit feature maps, KDD 2013

¹Charikar et al, Finding frequent items in data streams, 2002

Backup slides

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

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 $\Omega(m^{2.5})$
- 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

$$m \xrightarrow{m} \sqrt{m} \quad \overrightarrow{\Theta(m^{2.5})} \quad m \xrightarrow{m} \sqrt{m} \quad \overrightarrow{\Theta(m^{2})} \quad \overrightarrow{\Theta(m^{2.5})} \quad \overrightarrow{$$

- For the data with more tensors, we can derive the optimal way to sketch using the two-tensor scheme for a given contraction path
- ${\ensuremath{\, \bullet }}$ 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 embeddings¹

Efficient algorithms for tensors



¹Ahle et al, Oblivious sketching of high-degree polynomial kernels, SODA 2020

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 finder¹

- Generate a random embedding matrix $\Omega \in \mathbb{R}^{n imes \Theta(r)}$
- $Q, R \leftarrow \mathsf{qr}(A\Omega)$, so $Q \in \mathbb{R}^{m imes \Theta(r)}$

Dimensionality reduction

• $B \leftarrow Q^T A$

SVD on the low-rank matrix QB

- $Q_B, \Sigma, V_B^T \leftarrow \mathsf{svd}(B)$
- Return QQ_B, Σ, V_B^T



¹Nathan, Martinsson, and Tropp, Finding structure with randomness, SIAM review 2011

Efficient algorithms for tensors

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