Tensor Networks for Machine Learning

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Supervised Learning:

Learn $f: \mathcal{X} \to \mathcal{Y}$ from a sample $\{(x_1, y_1), \cdots, (x_N, y_N)\} \subset \mathcal{X} \times \mathcal{Y}$.

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 - ► Tensor structured data: Images, videos, spatio-temporal data, ...

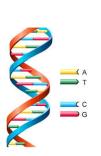


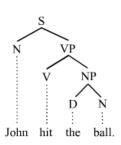
 $\in \mathbb{R}^{32 \times 32 \times 3} \simeq \mathbb{R}^{3072}$

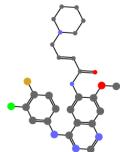
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- How to handle input/output structured data?
 - ► Tensor structured data: Images, videos, spatio-temporal data, ...
 - ▶ Discrete structured data: strings, trees, graphs, ...
- In both cases, one can leverage linear and tensor algebra to design learning algorithms.

Outline

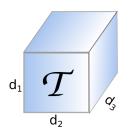
An Introduction to Tensors and Tensor Networks

- Tensor Networks for ML
 - Adaptive Learning of Tensor Decomposition Models
 - VC dimension of Tensor Network Models
 - Tensorized Random Projections

Tensors



$$\mathbf{M} \in \mathbb{R}^{d_1 imes d_2}$$
 $\mathbf{M}_{ij} \in \mathbb{R} ext{ for } i \in [d_1], j \in [d_2]$



$$\mathbf{M} \in \mathbb{R}^{d_1 \times d_2} \qquad \qquad \mathbf{\mathcal{T}} \in \mathbb{R}^{d_1 \times d_2 \times d_3}$$

$$\mathbf{M}_{ij} \in \mathbb{R} \text{ for } i \in [d_1], j \in [d_2] \qquad (\mathbf{\mathcal{T}}_{ijk}) \in \mathbb{R} \text{ for } i \in [d_1], j \in [d_2], k \in [d_3]$$

Tensors and Machine Learning

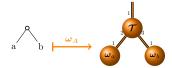
(i) Data has a tensor structure: color image, video, multivariate time series...





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(ii) Tensors as parameters of a model: polynomial regression, higher-order RNNs, weighted automata on trees and graphs...

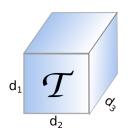


(iii) Tensors as tools: tensor method of moments [Anandkumar et al., 2014], layer compression in neural networks [Novikov et al., 2015], deep learning theoretical analysis [Cohen et al., 2015]...

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Tensors are not easy...

MOST TENSOR PROBLEMS ARE NP HARD

CHRISTOPHER J. HILLAR AND LEK-HENG LIM

ABSTRACT. The idea that one might extend numerical linear algebra, the collection of matrix computational methods that form the workhorse of scientific and engineering computing, to numerical multilinear algebra, an analogous collection of tools involving hypermatrices/tensors, appears very promising and has attracted a lot of attention recently. We examine here the computational tractability of some core problems in numerical multilinear algebra. We show that tensor analogues of several standard problems that are readily computable in the matrix (i.e. 2-tensor) case are NP hard. Our list here includes: determining the feasibility of a system of bilinear equations, determining an eigenvalue, a singular value, or the spectral norm of a 3-tensor, determining a best rank-1 approximation to a 3-tensor, determining the rank of a 3-tensor over $\mathbb R$ or $\mathbb C$. Hence making tensor computations feasible is likely to be a challenge.

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 \dots but training a neural network with 3 nodes is also NP hard [Blum and Rivest, NIPS '89]

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Forget rows and columns... Now we have **fibers**!

• Matrices have rows and columns, tensors have fibers¹:

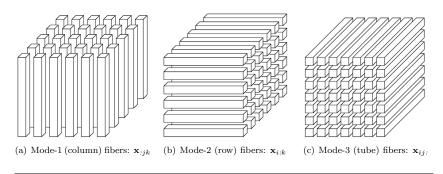
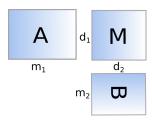


Fig. 2.1 Fibers of a 3rd-order tensor.

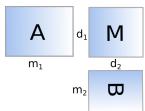
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¹fig. from [Kolda and Bader, Tensor decompositions and applications, 2009].

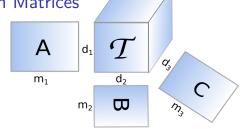
Tensors: Multiplication with Matrices



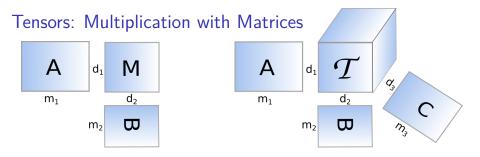




$$\mathsf{AMB}^ op \in \mathbb{R}^{m_1 imes m_2}$$



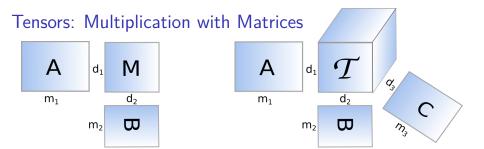
$$\mathcal{T} \times_1 \mathbf{A} \times_2 \mathbf{B} \times_3 \mathbf{C} \in \mathbb{R}^{m_1 \times m_2 \times m_3}$$



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ex: If $\mathcal{T} \in \mathbb{R}^{d_1 \times d_2 \times d_3}$ and $\mathbf{A} \in \mathbb{R}^{m_1 \times d_1}$, $\mathbf{B} \in \mathbb{R}^{m_2 \times d_2}$, $\mathbf{C} \in \mathbb{R}^{m_3 \times d_3}$, then $\mathcal{T} \times_1 \mathbf{A} \times_2 \mathbf{B} \times_3 \mathbf{C} \in \mathbb{R}^{m_1 \times m_2 \times m_3}$ is defined by



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$$(\mathcal{T} \times_1 \mathbf{A} \times_2 \mathbf{B} \times_3 \mathbf{C})_{i_1,i_2,i_3} = \sum_{k_1=1}^{n_1} \sum_{k_2=1}^{n_2} \sum_{k_2=1}^{n_3} \mathcal{T}_{k_1 k_2 k_3} \mathbf{A}_{i_1 k_1} \mathbf{B}_{i_2 k_2} \mathbf{C}_{i_3 k_3}$$

for all $i_1 \in [d_1], i_2 \in [m_2], i_3 \in [d_3].$

Degree of a node \equiv order of tensor





$$\mathbf{M} \in \mathbb{R}^{m imes n}$$



$$\mathcal{T} \in \mathbb{R}^{d_1 \times d_2 \times d_3}$$

Degree of a node \equiv order of tensor





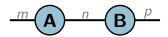
$$\mathbf{M} \in \mathbb{R}^{m \times n}$$

$$d_1$$
 d_3

$$\mathcal{T} \in \mathbb{R}^{a_1 \times a_2 \times a_3}$$

$$\mathsf{Edge} \equiv \mathsf{contraction}$$

Matrix product:



$$(\mathbf{AB})_{i_1,i_2} = \sum_{k=1}^n \mathbf{A}_{i_1 k} \mathbf{B}_{k i_2}$$

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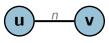
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Inner product:



$$\mathbf{u}^{\top}\mathbf{v} = \sum_{k=1}^{n} \mathbf{u}_{k} \mathbf{v}_{k}$$

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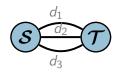


$$\mathsf{M} \in \mathbb{R}^{m imes n}$$

$$d_1$$
 d_3 d_3

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Inner product between tensors:



$$\langle \mathcal{S}, \mathcal{V}
angle = \sum_{i_1=1}^{d_1} \sum_{i_2=1}^{d_2} \sum_{i_3=1}^{d_3} \mathcal{S}_{i_1 i_2 i_3} \mathcal{T}_{i_1 i_2 i_3}$$

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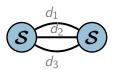


$$\frac{a_1}{\mathcal{T}} \underbrace{\mathcal{T}}_{a_3}$$

$$M \in \mathbb{R}^{m \times n}$$

$$\mathsf{Edge} \equiv \mathsf{contraction}$$

Frobenius norm of a tensor:



$$\|\mathcal{S}\|_F^2 = \sum_{i_1=1}^{d_1} \sum_{i_2=1}^{d_2} \sum_{i_3=1}^{d_3} (\mathcal{S}_{i_1 i_2 i_3})^2$$

Degree of a node \equiv order of tensor







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Trace of an $n \times n$ matrix:



$$\mathsf{Tr}(\mathsf{M}) = \sum_{i=1}^n \mathsf{M}_{ii}$$

Degree of a node \equiv order of tensor



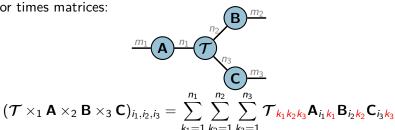




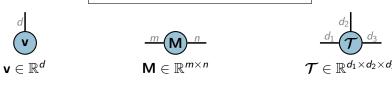
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 $Edge \equiv contraction$

Tensor times matrices:

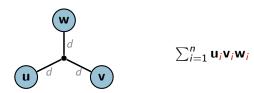


Degree of a node \equiv order of tensor



$$\mathsf{Edge} \equiv \mathsf{contraction}$$

Hyperedge \equiv contraction between more than 2 indices:



- Tensors can get huge quickly:
 - ▶ 3rd order tensor of shape $d \times d \times d$: d^3 parameters
 - ▶ 4th order tensor of shape $d \times d \times d \times d$: d^4 parameters
 - ▶ 10th order tensor of shape $d \times d \times \cdots \times d$: d^{10} parameters
 - **>** ...

Simple idea: decompose a tensor into product of small factors.

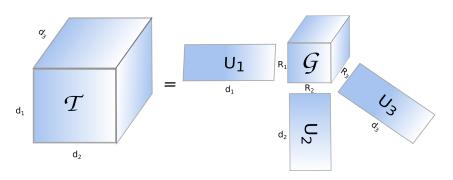
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- Similar to matrix factorization:
 - ▶ If $\mathbf{M} \in \mathbb{R}^{m \times n}$ and $\mathbf{M} = \mathbf{A}\mathbf{B}$ with $\mathbf{A} \in \mathbb{R}^{m \times r}$ and $\mathbf{B} \in \mathbb{R}^{r \times n}$

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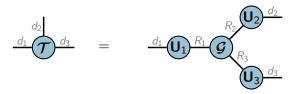
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 - $\Rightarrow r(m+n)$ parameters instead of mn...

• Tucker decomposition [Tucker, 1966]:



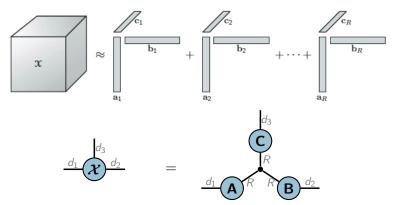
 \Rightarrow $R_1R_2R_3 + d_1R_1 + d_2R_2 + d_2R_2$ parameters instead of $d_1d_2d_3$.

• Tucker decomposition [Tucker, 1966]:



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• CP decomposition [Hitchcock, 1927]²:

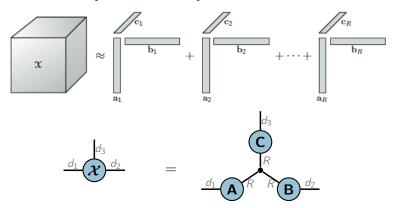


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²fig. from [Kolda and Bader, *Tensor decompositions and applications*, 2009].

• CP decomposition [Hitchcock, 1927]²:



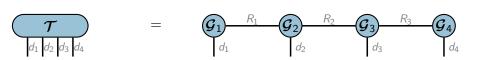
 \Rightarrow $R(d_1 + d_2 + d_3)$ parameters instead of $d_1d_2d_3$.

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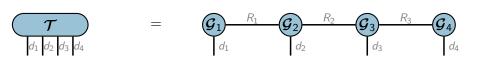
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• Tensor Train decomposition [Oseledets, 2011]:

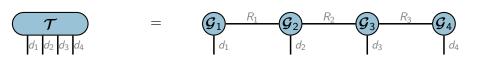


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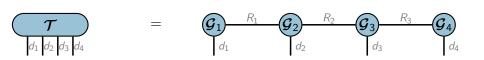
 $\Rightarrow d_1R_1 + R_1d_2R_2 + R_2d_2R_3 + R_3d_4$ parameters instead of $d_1d_2d_3d_4$.

Tensor Train decomposition [Oseledets, 2011]:



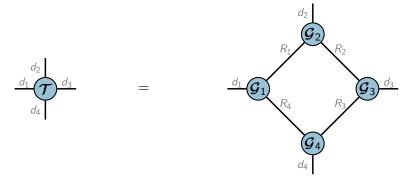
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 - If the ranks are all the same $(R_1 = R_2 = \cdots = R)$, can represent a vector of size 2^n with $\mathcal{O}(nR^2)$ parameters!

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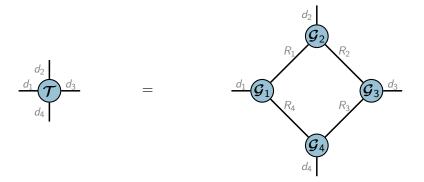


- $\Rightarrow d_1R_1 + R_1d_2R_2 + R_2d_2R_3 + R_3d_4$ parameters instead of $d_1d_2d_3d_4$.
 - If the ranks are all the same $(R_1 = R_2 = \cdots = R)$, can represent a vector of size 2^n with $\mathcal{O}(nR^2)$ parameters!
 - We can also efficiently perform operations on TT tensors:
 - Inner product, sum, component-wise product, ... all in time linear in n for vectors of size dⁿ.

• Tensor Ring decomposition [Zhao et al., 2016]:



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 \Rightarrow $R_4d_1R_1 + R_1d_2R_2 + R_2d_2R_3 + R_3d_4R_4$ parameters instead of $d_1d_2d_3d_4$.

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- \bullet Tensor decomposition \equiv efficient way to compress high dimensional objects
- \hookrightarrow can be used to compress neural networks (e.g., [Novikov et al., 2015])
- ⇒ Lots of interesting open problems and connections with quantum physics and formal languages.
- ⇒ Tensors are the new matrices (linear → multilinear) and tensor networks make it "easy" to reason about tensors, tensor decomposition and multi-linear algebra.

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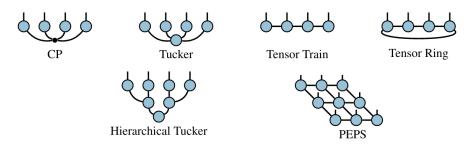
Joint work with Meraj Hashemizadeh, Michelle Liu and Jacob Miller







• Lots of ways to decompose a tensor:



- ⇒ How to choose the *right* decomposition model for a given ML problem?
- ⇒ Can we design adaptive algorithms, learning the decomposition structure from data?
- ⇒ What are the different implicit bias encoded in each decomposition model?

 $\Rightarrow \dots$

A lot of tensor problems can be formulated as

$$\min_{oldsymbol{\mathcal{W}} \in \mathbb{R}^{d_1 imes \cdots imes d_p}} L(oldsymbol{\mathcal{W}}) \quad ext{ s.t. } ext{ rank}(oldsymbol{\mathcal{W}}) \leq R$$

where L is a loss function and rank is some notion of tensor rank (e.g. TT, TR, CP, ...).

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► Tensor Decomposition

$$L(\mathcal{W}) = \|\mathcal{T} - \mathcal{W}\|_F^2$$

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► Tensor Classification

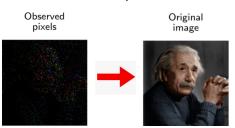
$$L(\mathcal{W}) = \sum_{i=1}^{N} \mathit{CCE}(y_i, f(\mathcal{X}_i))$$
 where $f(\mathcal{X}_i) = \mathrm{sign}(\langle \mathcal{W}, \mathcal{X}_i \rangle)$

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► Tensor Completion





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where L is a loss function and rank is some notion of tensor rank (e.g. TT, TR, CP, ...).

Tensor Completion

$$L(\mathcal{W}) = \sum_{(i,j,k) \in \Omega} (\mathcal{W}_{ijk} - \mathcal{X}_{ijk})^2$$

where Ω is the set of observed entries

A greedy algorithm for adaptive learning of TN structures

$$\min_{oldsymbol{\mathcal{W}} \in \mathbb{R}^{d_1 imes \cdots imes d_p}} \mathit{L}(oldsymbol{\mathcal{W}}) \quad ext{ s.t. } \mathsf{rank}(oldsymbol{\mathcal{W}}) \leq \mathit{R}$$

- We do not want to assume a fixed decomposition model.
- We want an algorithm that can adaptively find the best decomposition model for the task at hand.

A greedy algorithm for adaptive learning of TN structures

$$\min_{oldsymbol{\mathcal{W}} \in \mathbb{R}^{d_1 imes \cdots imes d_p}} L(oldsymbol{\mathcal{W}}) \quad ext{ s.t. } ext{ rank}(oldsymbol{\mathcal{W}}) \leq R$$

- We do not want to assume a fixed decomposition model.
- We want an algorithm that can adaptively find the best decomposition model for the task at hand.
- → We optimize the loss both with respect to the TN structure and the core tensors of the TN:

$$\min_{\text{Tensor Network Structure TN}} \min_{\boldsymbol{\mathcal{G}^{(1)}, \cdots, \mathcal{G}^{(p)}}} L(\mathit{TN}(\boldsymbol{\mathcal{G}^{(1)}, \cdots, \mathcal{G}^{(p)}}))$$
 s.t. $\mathtt{size}(\boldsymbol{\mathcal{G}^{(1)}, \cdots, \mathcal{G}^{(p)}}) \leq C$

A greedy algorithm for adaptive learning of TN structures

$$\min_{\text{Tensor Network Structure TN}} \min_{\mathcal{G}^{(1)}, \cdots, \mathcal{G}^{(p)}} L(TN(\mathcal{G}^{(1)}, \cdots, \mathcal{G}^{(p)}))$$
s.t. $\operatorname{size}(\mathcal{G}^{(1)}, \cdots, \mathcal{G}^{(p)}) \leq C$

- Pbm: the space of TN structures is exponentially large...
- We propose a simple greedy approach:
 - Start with a rank one tensor
 - Optimize the loss wrt the core tensors.
 - Greedily choose an edge to increment in the TN.
 - ▶ Repeat until the parameters budget is reached.

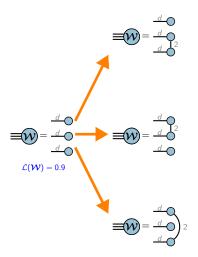
Start with a random rank one tensor.

$$= \underbrace{\frac{d}{d}}_{\underline{d}}$$

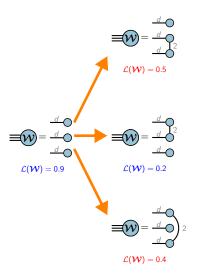
• Optimize the loss wrt the core tensors.



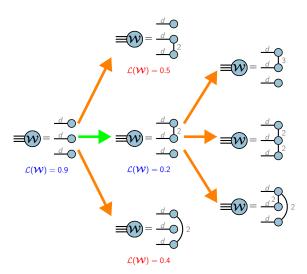
• Consider all possible rank one increments on internal edges.



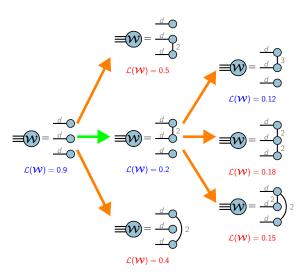
• Optimize the loss wrt core tensors for each possible increment.



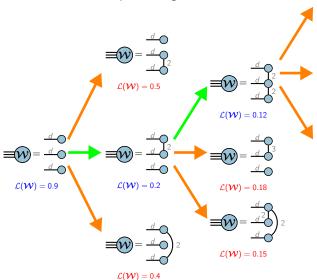
• Select the most promising rank increment and repeat...



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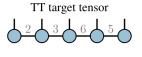


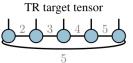
Implementation Details and Limitations

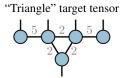
- At each iteration of greedy, we restart the optimization from the previous solution.
- No internal nodes are added to the initial TN structure (cannot represent Tucker).
- No hyperedge (cannot represent CP).
- Computationally expensive.

Experiment: Tensor decomposition

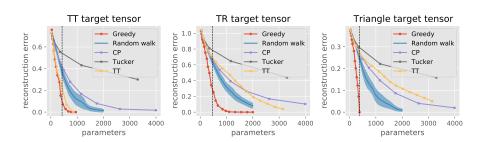
- Objective: compress a given tensor (with unknown tensor network structure) by decomposing it.
- Three target tensors of size $7 \times 7 \times 7 \times 7 \times 7$:



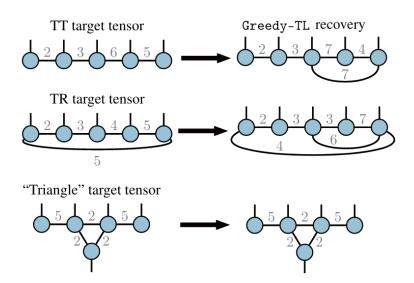




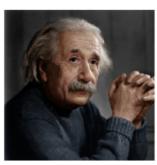
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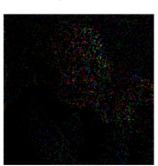
Tensor structures recovered by Greedy



Original image



Observed pixels

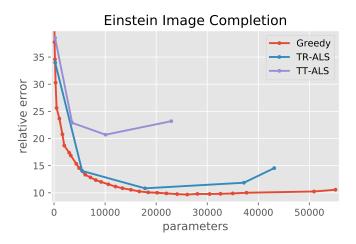


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 \bullet Initial image is reshaped into a $6\times10\times10\times6\times10\times3$ tensor



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Conclusion

- We propose a general adaptive learning algorithm for tensor problem
- First step towards algorithms for general TN rather than specific tensor decomposition models
- Experimental results are very encouraging

Conclusion

- We propose a general adaptive learning algorithm for tensor problem
- First step towards algorithms for general TN rather than specific tensor decomposition models
- Experimental results are very encouraging
- Future directions (ongoing):
 - Theory: convergence rate analysis
 - Add support for internal nodes and hyperedges
 - Beyond Greedy:
 - ★ develop heuristics for more efficient search
 - ★ backtracking (e.g. A* algorithm)
 - experiments on compressing neural networks

Outline

- An Introduction to Tensors and Tensor Networks
- Tensor Networks for ML
 - Adaptive Learning of Tensor Decomposition Models
 - VC dimension of Tensor Network Models
 - Tensorized Random Projections

Joint work with Behnoush Khavari



- Classification problem: Given
 - ▶ a sample $S = \{(x_1, y_1), \dots, (x_n, y_n)\} \subset \mathcal{X} \times \{-1, +1\}$ drawn i.i.d. from an unknown distribution D
 - lacktriangle a class of hypothesis $\mathcal{H}\subset\{-1,1\}^\mathcal{X}$
 - ightharpoonup a loss function ℓ

we want to find $h \in \mathcal{H}$ which minimizes the risk

$$R(h) = \mathop{\mathbb{E}}_{(x,y)\sim D} \ell(h(x),y)$$

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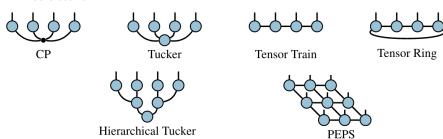
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 - ▶ the sample size *n*
 - the complexity of the hypothesis class \mathcal{H} .
- Many measures of complexity, here we focus on the VC dimension
 - ▶ $d_{VC}(\mathcal{H})$: maximum number of points that hypohtesis in \mathcal{H} can separate in all 2^n ways.

Problem

• We consider a classification problem with tensors:

$$R(h) = \sum_{i=1}^{n} \ell(y_i, h(\mathcal{X}_i))$$
 where $h(\mathcal{X}_i) = \operatorname{sign}(\langle \mathcal{W}, \mathcal{X}_i \rangle)$

and ${oldsymbol{\mathcal{W}}}$ is parameterized as a tensor network with an arbitrary structure



• Goal: Characterize the complexity of the hypothesis class \mathcal{H}_G for an arbitrary tensor network structure G.

Theorem

Let G = (V, E, dim) be a tensor network structure, let \mathcal{H}_G be the corresponding hypothesis class. The following hold:

• $d_{VC}(\mathcal{H}_G) \leq 2N_G \log(12|V|)$

where

- ullet N_G is the number of parameters in the tensor network
- ullet |V| is the number of vertices in the tensor network structure

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- $d_{VC}(\mathcal{H}_G) \leq 2N_G \log(12|V|)$
- For any $\delta > 0$, with probability at least 1δ over the choice of S, we have for any $h \in \mathcal{H}_G$

$$R(h) < \hat{R}_{\mathcal{S}}(h) + 2\sqrt{\frac{2}{n}}\left(N_{\mathcal{G}}\log\frac{8en|V|}{N_{\mathcal{G}}} + \log\frac{4}{\delta}\right).$$

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Discussion

- Our bound can be applied to any family of multilinear low rank classifiers, e.g. low rank matrix classifiers
- Our bound improves previous results in special cases (e.g. low rank matrices)
- Future work
 - lower bounds
 - structured risk minimization

Outline

- An Introduction to Tensors and Tensor Networks
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Joint work with Beheshteh T. Rakhshan, published at AISTATS 2020.



Motivation

- Random projection (RP) and tensor decomposition: Two tools to deal with high-dimensional data
- But RP cannot scale to very high-dimensional inputs (e.g. high-order tensors)
- We use tensor decomposition to scale Gaussian RP to high-order tensors

• Goal: find a low-dimensional projection $f: \mathbb{R}^d \to \mathbb{R}^k$ $(k \ll d)$ that preserves distances (with high proba.).

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- Johnson-Lindenstrauss Transform (or Gaussian RP).

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Theorem (JL, 1984)

Let $\varepsilon > 0$ and $\mathbf{x}_1, \dots, \mathbf{x}_m \in \mathbb{R}^d$. If $k \gtrsim \varepsilon^{-2} \log m$, then, with high proba., $\|f(\mathbf{x}_i)\| = (1 \pm \varepsilon) \|\mathbf{x}_i\|$ for all $i = 1, \dots, m$.

 Applications: sketched linear regression, randomized SVD, pre-processing step in ML pipeline, ...

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- Applications: sketched linear regression, randomized SVD, pre-processing step in ML pipeline, ...
- Pbm: if $\mathbf{x} \in \mathbb{R}^{d^N}$ is a high-order tensor represented in CP/TT format, the Gaussian RP has $d^N k$ parameters...

Objective

- We want to find a RP map $f: \mathbb{R}^{d^N} \to \mathbb{R}^k$ such that:
 - ▶ the number of parameters is linear in *N*
 - ightharpoonup computing f(x) is efficient when x is in the CP or TT format
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- Two important properties that a RP must satisfy:
 - $\mathbb{E}[\|f(\mathbf{x})\|^2] = \|\mathbf{x}\|^2$ for all **x**
 - $\qquad \qquad |\lim_{k\to\infty} \mathbb{V}[\|f(\mathbf{x})\|^2] = 0$
- \hookrightarrow the rate at which $\mathbb{V}[\|f(\mathbf{x})\|^2]$ converges to 0 captures the **quality** of a RP.

Tensor Train Random Projection (TT-RP)

• Tensor Train RP:

$$f_{TT(R)}: \mathbf{x} \mapsto \frac{1}{\sqrt{kR^N}} \mathbf{M} \mathbf{x}$$

where each row of $\mathbf{M} = \begin{pmatrix} -\mathbf{m}_1^\top - \\ -\mathbf{m}_2^\top - \\ \vdots \\ -\mathbf{m}_k^\top - \end{pmatrix} \in \mathbb{R}^{k \times d^N}$ is in the TT format:

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- $\mathcal{O}(kNdR^2)$ parameters instead of d^Nk .
- Efficient computation of Mx when x is in the CP/TT format.
- We have $\mathbb{E}[\|f_{TT(R)}(\mathbf{x})\|^2] = \|\mathbf{x}\|^2$.
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Theorem

Let $\mathbf{x} \in \mathbb{R}^{d^N}$ and $R \in \mathbb{N}$.

The RP maps $f_{TT(R)}$ and $f_{CP(R)}$ satisfy the following properties:

- $\mathbb{E}[\|f_{CP(R)}(\mathbf{x})\|^2] = \mathbb{E}[\|f_{TT(R)}(\mathbf{x})\|^2] = \|\mathbf{x}\|^2$
- $\mathbb{V}[\|f_{TT(R)}(\mathbf{x})\|^2] \le \frac{1}{k}(3(1+\frac{2}{R})^{N-1}-1)\|\mathbf{x}\|^4$
- $V[\|f_{CP(R)}(\mathbf{x})\|^2] \le \frac{1}{k} \left(3^{N-1} \left(1 + \frac{2}{R}\right) 1\right) \|\mathbf{x}\|^4$

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 \hookrightarrow The bounds on the variances are substantially different...

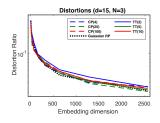
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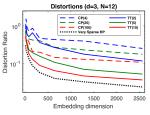
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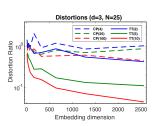
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- → The bounds on the variances are substantially different...
 - More details in paper on arXiv and Beheshteh's talk at AISTATS 2020.

Experiment Results







Discussion

- We proposed an efficient way to tensorize classical Gaussian RP
- Theory and experiments suggest that TT is better suited than CP for very high dimensional RP

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Discussion

- We proposed an efficient way to tensorize classical Gaussian RP
- Theory and experiments suggest that TT is better suited than CP for very high dimensional RP
- Future work:
 - ► Leverage results to design efficient linear regression and SVD algorithms
 - Beyond classical tensor decomposition: other TN structures better suited for RP?
 - Study of statistical properties of TT vectors with random Gaussian cores

Conclusion

- Forget matrices and linear algebra... Tensors and multilinear algebra!
- \bullet Tensor networks \equiv unifying language for tensor methods

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Thank you! Questions?