Tensor networks for machine learning: from random projections to learning the structure of tensor networks

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Supervised Learning:

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- Classical learning algorithms assume $\mathcal{X} = \mathbb{R}^d$ and $\mathcal{Y} = \mathbb{R}^p$.
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 - ► Tensor structured data: Images, videos, spatio-temporal data, ...



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

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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- How to handle input/output structured data?
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 - Discrete structured data: strings, trees, graphs, ...



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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

1 Preliminaries: Tensors and Multilinear Algebra

2 Tensorized Random Projections

3 Adaptive Learning of Tensor Decomposition Models

Tensors



$$\begin{split} \mathbf{M} \in \mathbb{R}^{d_1 \times d_2} & \mathcal{T} \in \mathbb{R}^{d_1 \times d_2 \times d_3} \\ \mathbf{M}_{ij} \in \mathbb{R} \text{ for } i \in [d_1], j \in [d_2] & (\mathcal{T}_{ijk}) \in \mathbb{R} \text{ for } i \in [d_1], j \in [d_2], k \in [d_3] \end{split}$$

Tensors and Machine Learning

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





(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]...

Tensors



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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 *numeri*cal 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.

[Hillar and Lim, Most tensor problems are NP-hard, Journal of the ACM, 2013.]

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

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.

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

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Tensor networks for ML



 $\mathbf{AMB}^{\top} \in \mathbb{R}^{m_1 \times m_2}$

 $\mathcal{T} imes_1 \mathbf{A} imes_2 \mathbf{B} imes_3 \mathbf{C} \in \mathbb{R}^{m_1 imes m_2 imes m_3}$



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ex: If $\mathcal{T} \in \mathbb{R}^{d_1 \times d_2 \times d_3}$ and $\mathbf{B} \in \mathbb{R}^{m_2 \times d_2}$, then $\mathcal{T} \times_2 \mathbf{B} \in \mathbb{R}^{d_1 \times m_2 \times d_3}$ and

$$(\mathcal{T} \times_2 \mathbf{B})_{i_1, i_2, i_3} = \sum_{k=1}^{d_2} \mathcal{T}_{i_1, k, i_3} \mathbf{B}_{i_2, k}$$
 for all $i_1 \in [d_1], i_2 \in [m_2], i_3 \in [d_3].$





Matrix product:





Inner product:

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



Trace of an $n \times n$ matrix:



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





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

▶ ...

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

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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 $d_1d_2d_3$.

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• CP decomposition [Hitchcock, 1927]²:



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

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Tensor networks for ML

• CP decomposition [Hitchcock, 1927]²:



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

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Tensor networks for ML

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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 (R₁ = R₂ = ··· = R), can represent a vector of size 2ⁿ with O (nR²) parameters!

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



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

Summary of Common Tensor Decomposition Models

- For an Nth order tensor of size $d \times d \times d \times \cdots \times d$, instead of d^N parameters we have
 - Tucker: $O(R^N + NdR)$ parameters
 - CP: O(NdR) parameters
 - Tensor train (TT): $O(NdR^2)$ parameters
 - Tensor ring (TR): $O(NdR^2)$ parameters

where the rank $R = \max_i R_i$.

Outline

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- 2 Tensorized Random Projections
- **3** Adaptive Learning of Tensor Decomposition Models

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

Random Projections (RP)

• 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).

$$f: \mathbf{x} \mapsto rac{1}{\sqrt{k}} \mathbf{M} \mathbf{x}$$
 where $\mathbf{M}_{ij} \sim_{iid} \mathcal{N}(0,1)$ for each i, j

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
 - computing $f(\mathbf{x})$ is efficient when \mathbf{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 \mathbf{x}
 - $\lim_{k\to\infty} \mathbb{V}[\|f(\mathbf{x})\|^2] = 0$

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- Two important properties that a RP must satisfy:
 - $\mathbb{E}[\|f(\mathbf{x})\|^2] = \|\mathbf{x}\|^2$ for all \mathbf{x}
- \hookrightarrow the rate at which $\mathbb{V}[[\|f(\mathbf{x})\|^2]$ converges to 0 captures the **quality** of a RP.

Tensor Train RP: First Attempt

• We build a Gaussian RP $f : \mathbf{x} \mapsto \frac{1}{Z}\mathbf{M}\mathbf{x}$ where $\mathbf{M} \in \mathbb{R}^{k \times d^N}$ is represented using the TT format:



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- $\bigcirc \mathcal{O}(R^2Nd + R^2k)$ parameters instead of d^Nk .
- \odot Efficient computation of **Mx** when **x** is in the CP/TT format.
- \bigcirc We have $\mathbb{E}[\|f(\mathbf{x})\|^2] = \|\mathbf{x}\|^2$.
- \odot We can show that $\lim_{k\to\infty} \mathbb{V}[\|f(\mathbf{x})\|^2] > 0...$

Tensor Train Random Projection (TT-RP): Second attempt

• Tensor Train RP:

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

where each row of $\mathbf{M} = \begin{pmatrix} -\mathbf{m}_1^T - \\ -\mathbf{m}_2^T - \\ \vdots \\ -\mathbf{m}_k^T - \end{pmatrix} \in \mathbb{R}^{k \times d^N}$ is in the TT format:
$$\underbrace{\mathbf{m}_i}_{d \ d \ d \ d} = \underbrace{\mathbf{G}_1^i}_{d \ d \ d} \underbrace{\mathbf{G}_2^i}_{d \ d \ d} \underbrace{\mathbf{G}_3^i}_{d \ d \ d} \underbrace{\mathbf{G}_4^i}_{d \ d \ d}$$
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- © $\mathcal{O}(kNdR^2)$ parameters instead of d^Nk .
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CP Random projection (CP-RP)

• CP Random Projection:

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

where each row of $\mathbf{M} = \begin{pmatrix} -\mathbf{m}_{1}^{T} - \\ -\mathbf{m}_{2}^{T} - \\ \vdots \\ -\mathbf{m}_{k}^{T} - \end{pmatrix} \in \mathbb{R}^{k \times d^{N}}$ is in the CP format:
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- CP Random projection (CP-RP)
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- $\bigcirc \mathcal{O}(kNdR)$ parameters instead of d^Nk .
- © Efficient computation of Mx when x is in the CP/TT format.
- [©] We have $\mathbb{E}[||f_{CP(R)}||^2] = ||\mathbf{x}||^2$.
- © We have $\lim_{k\to\infty} \mathbb{V}[\|f_{CP(R)}(\mathbf{x})\|^2] = 0...$

Main Result

Theorem

Let $\mathbf{x} \in \mathbb{R}^{d^N}$ and $R \in Ncal$. The RP maps $f_{TT(R)}$ and $f_{CP(R)}$ satisfy the following properties: • $\mathbb{E}[\|f_{CP(R)}(\mathbf{x})\|^2] = \mathbb{E}[\|f_{TT(R)}(\mathbf{x})\|^2] = \|\mathbf{x}\|^2$ • $\mathbb{V}[\|f_{TT(R)}(\mathbf{x})^2\|] \leq \frac{1}{k}(3\left(1+\frac{2}{R}\right)^{N-1}-1)\|\mathbf{x}\|^4$ • $\mathbb{V}[\|f_{CP(R)}(\mathbf{x})^2\|] \leq \frac{1}{k}\left(3^{N-1}\left(1+\frac{2}{R}\right)-1\right)\|\mathbf{x}\|^4$

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

Comparison between f_{CP} and f_{TT}

	$f_{CP(R)}: \mathbb{R}^{d^N} \to \mathbb{R}^k$	$f_{TT(R)}: \mathbb{R}^{d^N} \to \mathbb{R}^k$
Number of parameters	$\mathcal{O}(kNdR)$	$\mathcal{O}(kNdR^2)$
Computing $f(\mathbf{x})$ x in CP with rank $ ilde{R}$	$\mathcal{O}\left(k \textit{Nd} \max(r, ilde{R}^2 ight)$	$\mathcal{O}\left(kNd\max(r, ilde{R}^3 ight)$
Computing $f(\mathbf{x})$ x in TT with rank $ ilde{R}$	$\mathcal{O}\left(\textit{kNd}\max(r, ilde{R}^3 ight)$	$\mathcal{O}\left(kNd\max(r, ilde{R}^3 ight)$
With proba $\geq 1 - \delta$, $\mathbb{P}(\ f(\mathbf{x})\ ^2 = (1 \pm \varepsilon) \ \mathbf{x}\ ^2)$ as soon as $k \gtrsim \cdots$	$\frac{3^{N-1}(1+2/R)}{\varepsilon^2}\log^{2N}\left(\frac{1}{\delta}\right)$	$\frac{(1+2/R)^{N}}{\varepsilon^{2}}\log^{2N}\left(\frac{1}{\delta}\right)$

Comparison between f_{CP} and f_{TT}

	$f_{CP(R)}: \mathbb{R}^{d^N} \to \mathbb{R}^k$	$f_{TT(R)}: \mathbb{R}^{d^N} \to \mathbb{R}^k$
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Computing $f(\mathbf{x})$ x in TT with rank $ ilde{R}$	$\mathcal{O}\left(\textit{kNd}\max(r, ilde{R}^3 ight)$	$\mathcal{O}\left(kNd\max(r, ilde{R}^3 ight)$
$ \begin{array}{l} \text{With proba} \geq 1 - \delta, \\ \mathbb{P}(\ f(\mathbf{x})\ ^2 = (1 \pm \varepsilon) \ \mathbf{x}\ ^2) \\ \text{ as soon as } k \gtrsim \cdots \end{array} $	$\frac{3^{N-1}(1+2/R)}{\varepsilon^2}\log^{2N}\left(\frac{1}{\delta}\right)$	$\frac{(1+2/R)^{N}}{\varepsilon^{2}}\log^{2N}\left(\frac{1}{\delta}\right)$

- Lower bounds on k suggest that f_{TT} is a better RP than f_{CP} .
- Classical Gaussian RP needs $k \gtrsim \frac{1}{\varepsilon^2} \log \left(\frac{1}{\delta} \right)$.
- Comparisons with other approaches: see paper on arXiv and Beheshteh Rakhshan's talk at AISTATS 2020.

Experiment Setup

- Compare f_{TT}, f_{CP} and classical Gaussian RP to project d^N dimensional vectors
 - small order: d = 15, N = 3
 - medium order: d = 3, N = 12
 - higher order: d = 3, N = 25
- Input **x** is a random unit-norm TT vector with rank $\tilde{R} = 10$.
- Metric: distortion ratio $\frac{\|f(\mathbf{x})\|^2}{\|\mathbf{x}\|^2} 1$
- Report averages over 100 trials

Experiment Results



Conclusion

- We proposed an efficient way to tensorize classical Gaussian RP
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Conclusion

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- 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

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Joint work with Meraj Hashemizadeh, Michelle Liu and Jacob Miller







Tensor Decomposition Techniques

• Lots of ways to decompose a tensor:



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

 \Rightarrow

. . .

Tensor based optimization problems

• A lot of tensor problems can be formulated as

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

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

Tensor Decomposition

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

Tensor Regression

$$L(\mathcal{W}) = \|\mathcal{W} \times_1 \mathbf{X} - \mathcal{Y}\|_F^2$$

Tensor Completion

...

Matrix and tensor completion



figure credits: Heartbeat Fritz AI: Recommender systems with Python

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Matrix and tensor completion



• Here $L(\mathbf{W}) = \sum_{(i,j)\in\Omega} (\mathbf{W}_{i,j} - \mathbf{X}_{i,j})^2$ where Ω is the set of observed entries and the minimization problem is

$$\min_{\mathbf{W}\in\mathbb{R}^{n imes m}}L(\mathbf{W})$$
 s.t. $\mathrm{rank}(\mathbf{W})\leq k$

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which is equivalent to:

$$\min_{\mathbf{U}\in\mathbb{R}^{n\times k},\mathbf{V}\in\mathbb{R}^{k\times m}}L(\mathbf{UV})$$

figure credits: Heartbeat Fritz AI: Recommender systems with Python

A greedy algorithm for adaptive learning of TN structures

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- 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.

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- We want an algorithm that can adaptively find the best decomposition model for the task at hand.
- \hookrightarrow We optimize the loss both with respect to the TN structure and the core tensors of the TN:

 $\begin{array}{c} \min \\ \text{Tensor Network Structure TN} & \min_{\mathcal{G}^{(1)}, \cdots, \mathcal{G}^{(p)}} L(TN(\mathcal{G}^{(1)}, \cdots, \mathcal{G}^{(p)})) \\ \text{s.t. size}(\mathcal{G}^{(1)}, \cdots, \mathcal{G}^{(p)}) \leq C \end{array}$

A greedy algorithm for adaptive learning of TN structures

$$\begin{array}{c} \min\limits_{\text{Tensor Network Structure TN}} \min\limits_{\mathcal{G}^{(1)}, \cdots, \mathcal{G}^{(p)}} L(\mathit{TN}(\mathcal{G}^{(1)}, \cdots, \mathcal{G}^{(p)})) \\ \text{s.t. size}(\mathcal{G}^{(1)}, \cdots, \mathcal{G}^{(p)}) \leq C \end{array}$$

- 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.



• 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...



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


Greedy Algorithm Overview

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



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.
- Target tensors:





Experiment: Tensor decomposition



Experiment: Tensor completion

Original image



Observed pixels



Experiment: Tensor completion



Guillaume Rabusseau

Experiment: Tensor completion



Einstein Image Completion

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
- Related to the work of Chao Li and Zhun Sun at ICML 2020

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
- Related to the work of Chao Li and Zhun Sun at ICML 2020
- Future directions (ongoing):
 - Theory: we can show an exponential convergence rate to a solution achieving the optimal loss
 - 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

Thank you! Questions?