Flexible Tensor Decompositions for Learning and Optimization **Anand D. Sarwate, Rutgers University** 7 April 2025



IIIT-Hyderabad



Tensors: what are they good for?

All images: Wikipedia



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• 1913: Albert Einstein and Marcel Grossman used tensor calculus extensively in their work on general relativity: Entwurf einer verallgemeinerten Relativitätstheorie und einer Theorie der Gravitation

• 1915–17: Levi-Civita and Einstein have a correspondence where the former helped fix the mistakes in the use of tensor analysis.

 1922: H. L. Brose's English translation of Weyl's book Raum, Zeit, Materie (Space-Time-Matter) uses "tensor analysis."





 $\mathbf{x} \in \mathrm{R}^m$

First-Order Tensor (Vector)





First-Order Tensor (Vector)

 $\mathbf{X} \in \mathrm{R}^{m_1 imes m_2}$

Second-Order Tensor (Matrix)



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 $\mathbf{X} \in \mathbf{R}^{m_1 imes m_2}$ Second-Order Tensor (Matrix)



 $\mathbf{\underline{X}} \in \mathrm{R}^{m_1 imes m_2 imes m_3}$

Third-Order Tensor



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Third-Order Tensor

$$\mathbf{X} \in \mathbb{R}^{m_1 \times m_2 \times \cdots \times m_K}$$



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Third-Order Tensor

For this talk, I will treat treat tensors "computationally" as multidimensional arrays:

$$\underline{\mathbf{X}} \in \mathbb{R}^{m_1 \times m_2 \times \cdots \times m_K}$$

There are other (richer) perspectives:



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- There are other (richer) perspectives:
- Point in the tensor product of vector spaces



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- Point in the tensor product of vector spaces
- Multilinear operator



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- There are other (richer) perspectives:
- Point in the tensor product of vector spaces
- Multilinear operator
- Tensor representation of GL(n)











Medicine: Neuroimaging (and other kinds of imaging)











- Medicine: Neuroimaging (and other kinds of imaging)
- Geosensing: Hyperspectral imaging











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- Geosensing: Hyperspectral imaging
- Communications: Massive MIMO











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- Probability: Joint PMFs on multiple variables











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- Network science: Time-varying graphs











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- Geosensing: Hyperspectral imaging
- Communications: Massive MIMO
- Probability: Joint PMFs on multiple variables
- Network science: Time-varying graphs
- Also quantum physics, chemometrics, numerical linear algebra, psychometrics, theoretical computer science...





















- Signal recovery
- Supervised learning (prediction)




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- Signal recovery
- Supervised learning (prediction)
- Representation learning (compression)





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Task: given a collection of tensors $\underline{\mathbf{Y}}_1$ dictionary $\underline{\mathbf{d}}_1, \underline{\mathbf{d}}_2, \dots, \underline{\mathbf{d}}_p$ such that



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where each vector of coefficients \mathbf{X}_i =

Application: processing or storing hyperspectral images acquired from a drone.

rs
$$\underline{\mathbf{Y}}_1, \underline{\mathbf{Y}}_2, \dots, \underline{\mathbf{Y}}_n \in \mathbb{R}^{m_1 \times m_2 \times \dots \times m_K}$$
, find a
at
 $\underline{\mathbf{Y}}_i \approx \sum_{j=1}^p x_{ij} \underline{\mathbf{d}}_j$,
s $\mathbf{x}_i = (x_{i1}, x_{i2}, \dots, x_{ip})^{\top}$ is *s*-sparse.

Task: given a collection of tensor-scalar pairs $\{(\underline{\mathbf{X}}_i, y_i)\} \subset \mathbb{R}^{m_1 \times m_2 \times \cdots \times m_K} \times \mathbb{R}$, find a *regression tensor* **B** such that

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 $y_i \approx \langle \underline{\mathbf{B}}, \underline{\mathbf{X}}_i \rangle + \text{noise},$

where $\langle \cdot, \cdot \rangle$ is the element-wise inner product.

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$$,\underline{\mathbf{X}}_{i}
angle$$
 + noise,

Why not use large "foundation" models? For many applications, data is high-dimensional and expensive











Example: ADHD-200 sample aggregates 8 international imaging sites (US, Netherlands, China) with fMRI images of children's and adolescents' brains.

- fMRI data: 121 x 145 x 121 tensor
- After vectorizing: 2,122,945 dimensional vector
- Sample size: 959 total images











vectorize













Regression: 2.1m ViT-Huge: 632m



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- Matrices: model **B** as low rank.



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- Vectors: model **B** as sparse.
- Matrices: model **B** as low rank.
- **Tensors:** a lot more choices!





...

What's in this talk A preview of the rest of the talk

- 1. Tensor decompositions and where to find them
- 2. Supervised learning with LSR tensor structures
- 3. Some current and future directions

lensor decompositions (old and "new")

Some tensor terminology A little jargon is unavoidable...





Kolda and Bader (2009) Cichocki (2016) Sidiropolous et al. (2017)



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 m_2







- Mode: each coordinate index
- Order: the number of modes of the tensor
- Fibers: 1-D vectors along each mode





 m_{γ}











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 m_{γ}













- Mode: each coordinate index
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 m_{γ}







- Mode 1 = spectrum
- Mode 2 = longitude
- Mode 3 =latitude









Multiply a tensor $\mathbf{G} \in \mathbb{R}^{r_1 \times r_2 \times \cdots \times r_K}$ by a matrix $\mathbf{B}_k \in \mathbb{R}^{m_k \times r_k}$ along mode k: $\underline{\mathbf{G}} \times_k \mathbf{B}_k$





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The result is a order-K tensor whose k-th mode is m_k dimensional.



 m_1

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Matrix-tensor product example Filtering hyperspectral images







If $\underline{\mathbf{X}}$ is a hyperspectral image and \mathbf{L} is a Discrete Fourier Transform (DFT) matrix corresponding to a lowpass filter, then:

$\mathbf{X} \mathbf{X}_1 \mathbf{L}_1$

Applies the lowpass filter to the fiber (spectrum) at each physical location in space.







 $m_2 imes r_2$



We can change the shape of a tensor with repeated matrixtensor products



 $\underline{\mathbf{G}} \times_1 \mathbf{B}_1 \times_2 \mathbf{B}_2 \cdots \times_K \mathbf{B}_K = \mathbf{X} \in \mathbb{R}^{m_1 \times m_2 \cdots \times m_K}$

Tensor Rank(s) and Tensor Decompositions/Factorizations

• 2D: a rank-1 matrix



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- 2D: a rank-1 *matrix*
- rank-r matrix can be written as the sum of r rank-1 matrices.
- A matrix has a CANDECOMP/ **PARAFAC (CP)** representation of order r if we can write it as a sum of *r* rank-1 outer products.





CP Decomposition

CP factorization Writing the decomposition with matrix-tensor products



Gather the factors from each mode into matrices and define an $r \times r \times \cdots \times r$ diagonal core tensor <u>G</u>:

$\underline{\mathbf{B}}_{\mathsf{CP}} = \underline{\mathbf{G}} \times_1 \mathbf{I}$

The total number of parameters is r(1 +

$$\mathbf{B}_{1} \times_{2} \mathbf{B}_{2} \cdots \times_{K} \mathbf{B}_{K}$$
$$\sum_{k=1}^{K} m_{k} \text{) as opposed to } \prod_{k=1}^{K} m_{k}.$$

Tucker decomposition Filling out the core tensor





Tucker decomposition Filling out the core tensor

 $m_2 imes r_2$ and expand the dimensions using matrix-tensor products. This is the **Tucker decomposition**: \mathbf{B}_2 $m_3 imes r_3$ $m_1 imes r_1$ The total number of parameters is G \mathbf{B}_3 \mathbf{B}_1 $r_1 imes r_2 imes r_3$



Suppose we have a **core tensor**

$$\underline{\mathbf{G}} \in \mathbb{R}^{r_1 \times r_2 \times \cdots \times r_K}$$

$$\underline{\mathbf{B}}_{\mathsf{Tucker}} = \underline{\mathbf{G}} \times_1 \mathbf{B}_1 \times_2 \mathbf{B} \times_3 \mathbf{B}_3$$

$$\prod_{k=1}^{K} r_k + \sum_{k=1}^{K} m_k r_k$$

Other tensor decompositions A plethora of options

There are other tensor decompositions out there (see Cichocki 2016):

- Tensor Train
- Hierarchical Tucker/Tree Tensor Network States

Kolda and Bader 2009), which can written as a **mixture of Tucker models**:

$$\underline{\mathbf{B}}_{\mathsf{BTD}} = \sum_{s=1}^{S} \underline{\mathbf{G}}_{s} \times_{1} \mathbf{B}_{1,s} \times_{2} \mathbf{B}_{2,s} \cdots \times_{K} \mathbf{B}_{K,s},$$

each $s \in [S]$. We will assume a common **G** for all terms.

Our proposal is to use a simpler form of a **block tensor decomposition** (Section 5.7,

In general, each \underline{G}_{s} can have a different size, so we need to choose S and $\{m_{k,s}, r_{k,s}\}$ for

Issues with decompositions There are many different definitions of "rank" for tensors

- **CP** rank of $\underline{\mathbf{B}}$ = smallest number of terms in a CP decomposition (Hitchcock 1927, Kruskal 1977).
 - 👍 The decomposition is (often) unique.
 - F Computing the rank is NP-complete for finite fields and NP-hard for Q (Håstad 1990, resolving a conjecture of Gonzalez and Ja'Ja' 1980).
- **Tucker rank** is a **vector**. Decomposition can be computed using the higherorder SVD [HOSVD] or other algorithms (De Lathauwer et al. 2000, also others).
 - Tucker rank is **not** unique.

Matrix Equivalents of Tensor Factorizations

A different kind of vectorization Matrix-tensor products as matrix vector products



Start with a Tucker factorization:

$$\underline{\mathbf{B}}_{\mathsf{Tucker}} = \underline{\mathbf{G}} \times_1 \mathbf{B}_1 \times_2 \mathbf{B}_2 \cdots \times_K \mathbf{B}_K$$

- If we vectorzize $\underline{B}_{\mathsf{Tucker}}$, we get get the following equivalent model:
 - $\operatorname{vec}(\underline{\mathbf{B}}_{\mathsf{Tucker}}) = (\mathbf{B}_K \otimes \cdots \otimes \mathbf{B}_1) \operatorname{vec}(\underline{\mathbf{G}})$
- where \otimes is the Kronecker product.

The Kronecker product Matrix-tensor products as a matrix vector product

The Kronecker product makes "copies" of one matrix inside the other: $\mathbf{A} \otimes \mathbf{B} = \begin{bmatrix} a_{11} \\ \vdots \\ a_{m1} \end{bmatrix}$

Vectorizing shows that the Tucker decomposition

$$\operatorname{vec}(\underline{\mathbf{B}}_{\mathsf{Tucker}}) = (\mathbf{B}_{K})$$

Is somewhat restrictive.

B	• • •	$a_{1n}\mathbf{B}$
• •	•••	• • •
$n^{1}\mathbf{B}$	• • •	$a_{mn}\mathbf{B}$

 $\otimes \cdots \otimes \mathbf{B}_2 \otimes \mathbf{B}_1$ vec(**G**)

BTD with a common core tensor



Special case of the BTD is a low separation rank (LSR) decomposition:

$$\underline{\mathbf{B}}_{\mathsf{LSR}} = \sum_{s=1}^{S} \underline{\mathbf{G}} \times_1 \mathbf{B}_{1,s} \times_2 \mathbf{B}_{2,s} \cdots \times_K \mathbf{B}_{K,s}$$

We use the same core tensor G for each term. We also assume that the factor matrices $\{\mathbf{B}_{k,s}\}$ have orthonormal columns.



What does separation rank mean? Writing matrices as sums of Kronecker products

The separation rank (Tsiligkaridis and Hero, 2013) of a matrix is the minimum number S of terms needed so that

$$\mathbf{M} = \sum_{s=1}^{S} \mathbf{A}_{K,s}$$

Our LSR model corresponds assuming the matrix-vector product has a matrix with low separation rank

$$\sum_{s=1}^{S} \underline{\mathbf{G}} \times_{1} \underline{\mathbf{B}}_{1,s} \times_{2} \underline{\mathbf{B}}_{2,s} \cdots \times_{K} \underline{\mathbf{B}}_{K,s} = \underline{\mathbf{B}}_{\mathsf{LSR}} \Longrightarrow \left(\sum_{s} \bigotimes_{k} \mathbf{B}_{k}\right) \mathbf{g}$$

$$\otimes \cdots \otimes \mathbf{A}_{2,s} \otimes \mathbf{A}_{1,s}$$

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- Tucker + logistic regression (Zhang et al. 2016)
- Tucker + GLMs (Li et al., 2018; Zhou et al., 2013)

The benefits of more flexible modeling Taking advantage of more data



LSR models let use scale the number of parameters to the data set size.

Synthetic data experiments show that with a modest number of samples, LSR models are better than vectorizing or using a Tucker model.

Comparing different decompositions







Regression and classification with LSR tensors

family:

$$p(y;\eta) = b(y) \exp\left(-\eta T(y) - a(\eta)\right).$$

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Where the parameter $\eta = \langle \mathbf{B}, \mathbf{X} \rangle$. One example is *logistic regression*:

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$$\frac{1}{1 + \exp(-\langle \mathbf{\underline{B}}, \mathbf{\underline{X}} \rangle)}$$

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Our goal: estimate **B**.

$$\frac{1}{1 + \exp(-\langle \mathbf{\underline{B}}, \mathbf{\underline{X}} \rangle)}$$

Estimation in GLMs using LSR Tensors

Mapping the tensor to a matrix Using the LSR matrix in the vectorized problem

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Under an LSR model, we have

$$\eta = \left\langle \sum_{s=1}^{S} \underline{\mathbf{G}} \times_{1} \mathbf{B}_{(1,s)} \right\rangle$$

 $\times_2 \mathbf{B}_{(2,s)} \times_3 \cdots \times_K \mathbf{B}_{(K,s)}, \underline{\mathbf{X}} \right\rangle$

Mapping the tensor to a matrix Using the LSR matrix in the vectorized problem

Under an LSR model, we have

$$\eta = \left\langle \sum_{s=1}^{S} \mathbf{\underline{G}} \times_{1} \mathbf{B}_{(1,s)} \right\rangle$$

Vectorizing:

$$\eta = \left\langle \left(\sum_{s=1}^{S} \mathbf{B}_{(K,s)} \otimes \mathbf{B} \right) \right\rangle$$



Maximum likelihood estimator (MLE) Sorry, but it's a bit messy...

The MLE comes from minimizing

Over all $\mathbf{B}_{k,s} \in \mathbb{O}^{m_k \times r_k}$ and $\mathbf{g} \in \mathbb{R}^{r_1 r_2 \cdots r_K}$. In practice this is not a nice optimization so we use alternating minimization on $\{\mathbf{B}_{(k,s)}\}$ and \mathbf{g} .

Question: does the MLE work and is it optimal?

 $\sum_{i=1}^{n} \left| \left\langle \left(\sum_{s=1}^{S} \bigotimes_{k} \mathbf{B}_{(k,s)} \right) \mathbf{g}, \mathbf{x}_{i} \right\rangle T(y_{i}) - a \left(\left\langle \left(\sum_{s=1}^{S} \bigotimes_{k} \mathbf{B}_{(k,s)} \right) \mathbf{g}, \mathbf{x}_{i} \right\rangle \right) \right| \right|$

Space of LSR models **Counting parameters**

Suppose we are given $(r_1, r_2, \ldots, r_K, S)$. Then define

where for each (k, s), the columns of $\mathbf{B}_{(k,s)}$ are orthonormal.

Statistical/ML problems boil down to finding a "good" $\underline{\mathbf{B}} \in \mathscr{C}_{|SR}$.

$\mathscr{C}_{\mathsf{LSR}} = \left\{ \underline{\mathbf{B}} : \underline{\mathbf{B}} = \sum_{s=1}^{S} \underline{\mathbf{G}} \times_{1} \mathbf{B}_{(1,s)} \times_{2} \cdots \times_{K} \mathbf{B}_{(K,s)} \right\},\$

Question: does the # of parameters are $S \sum m_k r_k + \prod r_k$ capture the complexity? k



Packings: find a large set of points in \mathscr{C}_{LSR} which are a packing in the Frobenius norm $\|\cdot\|_{F}$.

- $\|\cdot\|_{F^{\bullet}}$

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Construction inspired by superposition codes (a bit) plus Gilbert-Varshamov coding.

- Packings: find a large set of points in \mathscr{C}_{LSR} which are a packing in the Frobenius norm $\|\cdot\|_{F^*}$
 - Construction inspired by superposition codes (a bit) plus Gilbert-Varshamov coding.
- **<u>Coverings</u>**: find a small set of ϵ -balls in $\|\cdot\|_F$ which cover \mathscr{C}_{LSR} .

- **Packings:** find a large set of points in \mathscr{C}_{ISR} which are a packing in the Frobenius norm $\|\cdot\|_{F^{\bullet}}$
 - Construction inspired by superposition codes (a bit) plus Gilbert-Varshamov coding.

<u>**Coverings:</u>** find a small set of ϵ -balls in $\|\cdot\|_F$ which cover $\mathscr{C}_{|SR}$.</u>

- Glue together coverings for the factors \underline{G} and (orthogonal) $\{\underline{B}_{(k,s)}\}$.

- **Packings:** find a large set of points in \mathscr{C}_{ISR} which are a packing in the Frobenius norm $\|\cdot\|_{F^{\bullet}}$
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Results: we get sets of the right size...

- $\|\cdot\|_{F^{\bullet}}$

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• Glue together coverings for the factors $\underline{\mathbf{G}}$ and (orthogonal) $\{\underline{\mathbf{B}}_{(k,s)}\}$.

Results: we get sets of the right size...

 $\approx \exp\left(S\right)$

Packings: find a large set of points in \mathscr{C}_{ISR} which are a packing in the Frobenius norm

Construction inspired by superposition codes (a bit) plus Gilbert-Varshamov coding.

$$\sum_{k} m_k r_k + \prod_{k} r_k \right)$$

Identifiability using MLE Sorry, but it's a bit messy...

$$n > \frac{C}{\epsilon^2} \left(\left(S \sum_k m_k r_k + \prod_k r_k \right) \log \left(\frac{C'}{\epsilon} \right) + \log \left(\frac{1}{\delta} \right) \right),$$

larger than ϵ .



Suppose $\{(\underline{\mathbf{X}}_{i}, y_{i}) : i \in [n]\} \subset \mathbb{R}^{m_{1} \times m_{2} \times \cdots \times m_{K}} \times \mathbb{R}$ are generated from a GLM with an LSR-structured parameter $\underline{\mathbf{B}}^{*}$. Then if

with probability $1 - \delta$ the MLE will find a model $\hat{\mathbf{B}}$ with excess risk no

A general lower bound for GLM + LSR After much fun with algebra...

$$\mathbb{E}\left[\left\|\underline{\mathbf{B}}^{*}-\underline{\hat{\mathbf{B}}}\right\|_{F}^{2}\right] = \Omega\left(\frac{S\sum_{k}(m_{k}-1)r_{k}+\prod_{k}(r_{k}-1)-1}{\left\|\boldsymbol{\Sigma}_{x}\right\|_{2}n}\right)$$

We can specialize this result to the Tucker and CP cases as well.

Suppose our data was generated with an LSR tensor \underline{B}^* We have a lower bound on the MSE for *any estimator* of \underline{B}^* :

(Taki, Sarwate, Bajwa, 2023)





Structure of $\underline{\mathbf{B}}$

Tucker

 \mathbf{LSR}



n

(Zhang et al., 2020)

$$\frac{-r}{n} \qquad \qquad \frac{\sum\limits_{k \in [K]} m_k r_k + \widetilde{r}}{M \| \boldsymbol{\Sigma}_x \|_2 n} \qquad \qquad \frac{S \sum\limits_{k \in [K]} m_k r_k + \widetilde{r}}{M \| \boldsymbol{\Sigma}_x \|_2 n}$$

$$2 \qquad \qquad \text{Corollary 1} \qquad \qquad \text{Theorem 6}$$

 \widetilde{r}

Experiments and applications

Experiments on medical imaging data **Data sets and algorithms**

(Yang et al., 2020).

Other algorithms:

- **TTR**: Tucker + GLMs using a 'block relaxation' algorithm (Li et al., 2018)
- LTuR: Tucker + logistic regression with Frobenius norm regularization (Zhang & Jiang, 2016)
- LR: Unstructured + logistic regression (Seber & Lee, 2003)
- LCPR: CP + logistic regression (Tan et al., 2013)

Data sets: ABIDE Autism [fMRI] (Craddock et al., 2013 2020), Vessel MNIST 3D [MRA]

ABIDE Autism data set A tiny data set: K = 2, m = (111, 116), n = 80

	\mathbf{SVM}
Sensitivity	0.71
Specificity	0.14
F1 score	0.55
\mathbf{AUC}	0.42
Average Accuracy	0.43

- Chose ranks $r_1 = 6$ and $r_2 = 6$ with S = 2.
- Unstructured models are quite bad in the undersampled regime.
- Adding one more Tucker component can give significant improvements.



\mathbf{LR}	LCPR	LTuR	LSRTR
0.71	0.71	0.71	1
0.71	0.85	0.85	0.85
0.71	0.77	0.77	0.93
0.51	0.84	0.84	0.9
0.71	0.78	0.78	0.92

VesselMNIST 3D **Comparing against a DNN too:** K = 3, r = (28, 28, 28), n = 1335

	\mathbf{SVM}	\mathbf{LR}	LCPR	LTuR	LSRTR	ResNet 50 + 3D
Sensitivity	0.39	0.53	0.26	0.32	0.47	0.85
Specificity	0.95	0.55	0.946	0.94	0.96	0.86
$\mathbf{F}1 \ \mathbf{score}$	0.44	0.21	0.3	0.37	0.55	0.57
\mathbf{AUC}	0.84	0.52	0.6	0.66	0.81	0.9
Average Accuracy	0.89	0.55	0.869	0.87	0.91	0.85

- Chose ranks $r_1 = 3$, $r_2 = 3$, $r_3 = 3$, and S = 2
- LSRTR has better accuracy but worse F1 and AUC (see paper).
- Issues such as overfitting, interpretability, etc. are still open.

Recap and looking forward

Recap of what we've seen Structuring tensors using factorizations for simpler modeling



- There is a whole continuum of tensor decompositions and LSR structured tensors can be very useful:
- Adapt parameterization to the data available.
- Efficiently (empirically) learnable/estimatable.

Other uses for LSR structures Some past, current, and ongoing directions

Dictionary learning: theory and algorithms



- Structuring latent space representations for generative models
- Reducing training and compute time

Even a KS assumption can help Even better results with LSR models (S > 1)



Original Image

Noisy Image

Unstructured DL: 147456 parameters

Separable DL: 265 parameters

Many questions remain! Lots to understand on the theory and practical side
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- Algorithms for computing decompositions with good guarantees for approximation and denoising.
- Convex relaxations of LSR constraint for optimization (we have some for dictionary learning!)
- Random tensor theory and spectral analysis.

Many questions remain! Lots to understand on the theory and practical side



- Algorithms for computing decompositions with good guarantees for approximation and denoising.
- Convex relaxations of LSR constraint for optimization (we have some for dictionary learning!)
- Random tensor theory and spectral analysis.



- More "real" applications in neuroimaging and other domains.
- Other data domains: hyperspectral imaging, chemometrics, etc.
- Information theoretic modeling.

