Analyzing identifiability of sparse linear networks

GdR ISIS - Theory of deep learning

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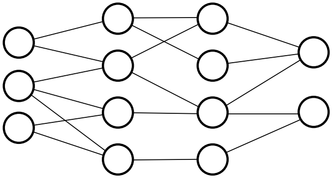
Sparse (linear) neural networks

- Reduce time + space complexity
- Toward interpretable NN?

→ requires identifiability / stability



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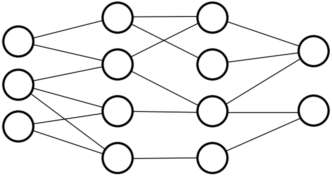

Analogy with NMF

Identifiability ensures that solution to NMF can be interpreted as the physical ground-truth.

Example: blind hyperspectral unmixing.

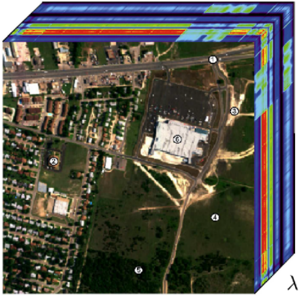

Figure: from [Gillis 2020]

Well-posedness in sparse matrix factorization?

Given a matrix $\boldsymbol{Z}$, and $L \geq 2$, solve

$$\min_{\boldsymbol{X_1},\dots,\boldsymbol{X_L}} \|\boldsymbol{Z} - \boldsymbol{X_L}\boldsymbol{X_{L-1}}\dots\boldsymbol{X_1}\|$$
$$\text{such that} \quad \boldsymbol{X_\ell} \text{ is } \textit{sparse}, \quad \forall \ell \in \{1, \dots, L\},$$

by exploring a given family of supports, with proximal algorithm [Le Magoarou and Gribonval 2016].

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Well-posedness of the problem is the key to recovery success:

- **uniqueness** of the solution to recover
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Focus on uniqueness in **exact** sparse matrix factorization → identifiability

Identifiability in exact sparse matrix facotrization

Outline

1. Analysis with two factors
2. Multilayer case via hierarchical factorization method

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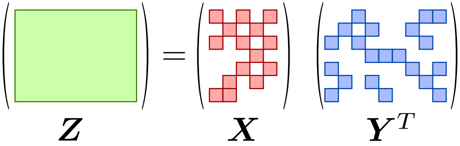
Given a matrix $\boldsymbol{Z}$ and a feasible set $\Sigma^L \times \Sigma^R$ of pairs of factors, define:

$$\text{find, if possible, } (\boldsymbol{X}, \boldsymbol{Y}) \in \Sigma^L \times \Sigma^R \text{ such that } \boldsymbol{Z} = \boldsymbol{X}\boldsymbol{Y}^T. \qquad \text{(EMF)}$$



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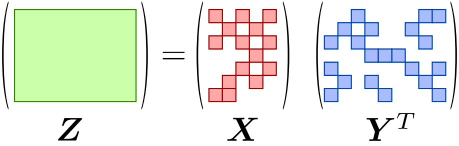

Informal Theorem

Let $\boldsymbol{Z}$ be a matrix, and $\Sigma^L \times \Sigma^R$ encoding sparsity on pairs of factors. If a certain condition on $\Sigma^L \times \Sigma^R$, then $\boldsymbol{Z}$ admits a unique EMF $\boldsymbol{Z} = \boldsymbol{X}\boldsymbol{Y}^T$ in $\Sigma^L \times \Sigma^R$, up to scaling and permutation ambiguities.

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Theorem

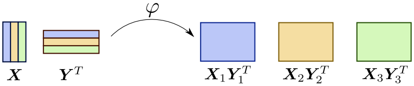
Let $\boldsymbol{Z}$ be the DFT, DCT-II or DST-II matrix of size $N = 2^L$. Suppose that:

- *Σ^L enforces 2-sparsity by column;*
- *Σ^R enforces $\frac{N}{2}$-sparsity by column.*

Then, $\boldsymbol{Z}$ admits a unique EMF $\boldsymbol{Z} = \boldsymbol{X}\boldsymbol{Y}^T$ in $\Sigma^L \times \Sigma^R$, up to scaling and permutation ambiguities.

Notation: $\Sigma^2_{\texttt{col}} \times \Sigma^{N/2}_{\texttt{col}}$.

Matrix decomposition into sparse rank-one matrices



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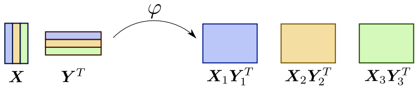

Given a matrix $\mathbf{Z}$ and a feasible set Γ of r-tuples of rank-one matrices, define:

$$\text{find, if possible, } (\mathcal{C}^i)_{i=1}^r \in \Gamma \text{ such that } \mathbf{Z} = \sum_{i=1}^{r} \mathcal{C}^i. \qquad \text{(EMD)}$$

$\rightarrow$ lifting procedure [Choudhary and Mitra 2014], [Le Magoarou 2016]

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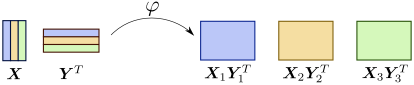

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Proposition

When $(\boldsymbol{X}, \boldsymbol{Y})$ is non-degenerate, identifiability of $(\boldsymbol{X}, \boldsymbol{Y})$ for the EMF of $\boldsymbol{Z} := \boldsymbol{X}\boldsymbol{Y}^T$ in $\Sigma^L \times \Sigma^R$ is equivalent to identifiability of $\varphi(\boldsymbol{X}, \boldsymbol{Y})$ for the EMD of $\boldsymbol{Z}$ in Γ.

In the case of $\Sigma^2_{\texttt{col}} \times \Sigma^{N/2}_{\texttt{col}}$:

$$\Gamma^{2,N/2} := \left\{ (\mathcal{C}^i)_{i=1}^r \mid \mathcal{C}^i \text{ has 2 nonzero rows, } \frac{N}{2} \text{ nonzero columns} \right\}.$$

Fixed-support identifiability

Analogy with sparse linear recovery (recover s-sparse $\boldsymbol{x}$ from $\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}$):

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$$\begin{pmatrix} 0 & 1 & 2 & 0 \\ 1 & 2 & 2 & 0 \\ 2 & 6 & 5 & 6 \\ 3 & 5 & 2 & 4 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ ? & ? & 0 & 0 \\ ? & ? & 0 & 0 \\ ? & ? & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & ? & ? & 0 \\ 0 & ? & ? & 0 \\ 0 & ? & ? & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & ? & ? & ? \\ 0 & ? & ? & ? \end{pmatrix}$$

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Remark: condition verified when the rank-one supports are disjoint.

Identifying the support constraint

Proposition

Let $\boldsymbol{Z}$ be the DFT, DCT-II or DST-II matrix. Then, for any EMD $\boldsymbol{Z} = \sum_{i=1}^{r} \boldsymbol{\mathcal{C}}^i$ with $\mathcal{C} \in \Gamma^{2,N/2}$, there exists σ such that: $\mathrm{supp}(\boldsymbol{\mathcal{C}}^i) \subseteq \boldsymbol{\mathcal{S}}^{\sigma(i)}$, where $\{\boldsymbol{\mathcal{S}}^i\}_{i=1}^r$ are pairwise disjoint.

$$\boldsymbol{DFT_4} = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & i & -1 & -i \\ 1 & -1 & 1 & -1 \\ 1 & -i & -1 & i \end{pmatrix}$$

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2. Only one possible partition $\{\boldsymbol{\mathcal{S}}^i\}_{i=1,2,3,4}$ of $\mathrm{supp}(\boldsymbol{DFT_4})$ such that $(\boldsymbol{DFT_4})_{|\boldsymbol{\mathcal{S}}^i}$ is of rank one.

Multilayer extension, with a butterfly sparsity structure

Given a matrix $\boldsymbol{Z}$ and a feasible set Σ of L-tuple of factors, define:

$$\text{find, if possible, } (\boldsymbol{X}_\ell) \in \Sigma \text{ such that } \boldsymbol{Z} = \boldsymbol{X}_{\boldsymbol{L}} \boldsymbol{X}_{\boldsymbol{L-1}} \ldots \boldsymbol{X}_{\boldsymbol{1}}. \qquad \text{(MEMF)}$$

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Here: $\Sigma^{\text{fly}} := \{\boldsymbol{X_L}, ..., \boldsymbol{X_1} \text{ have supp included in the butterfly supports}\}$.

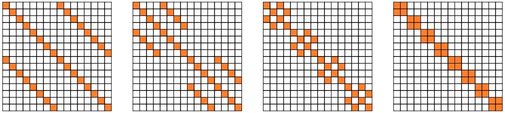

Figure: Butterfly supports: block diagonal + 2-sparse by row and by column.

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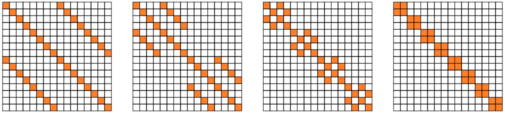

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Theorem

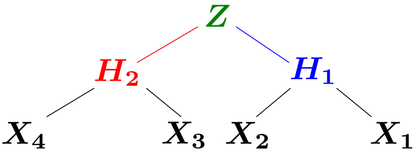
Let $\boldsymbol{Z} := \boldsymbol{X}_{\boldsymbol{L}} \boldsymbol{X}_{\boldsymbol{L-1}} \ldots \boldsymbol{X}_{\boldsymbol{1}}$ of size $N = 2^L$ where $\text{supp}(\boldsymbol{X}_{\boldsymbol{L}}), \ldots, \text{supp}(\boldsymbol{X}_{\boldsymbol{1}})$ are exactly the butterfly supports. Then, the factors $\boldsymbol{X}_{\boldsymbol{L}}, \ldots, \boldsymbol{X}_{\boldsymbol{1}}$ are the unique MEMF of $\boldsymbol{Z}$ in Σ^{fly}, up to scaling ambiguities.

Application: $\boldsymbol{Z}$ = DFT matrix of size $N = 2^L$.

A hierarchical factorization method

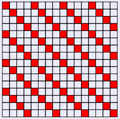
Consider $(\boldsymbol{X}_4, \boldsymbol{X}_3, \boldsymbol{X}_2, \boldsymbol{X}_1) \in \Sigma^{\text{fly}}$, and

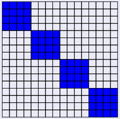
$$\boldsymbol{Z} = \boldsymbol{X}_4 \boldsymbol{X}_3 \boldsymbol{X}_2 \boldsymbol{X}_1.$$



Lemma

For any $(\boldsymbol{X}'_4, \boldsymbol{X}'_3, \boldsymbol{X}'_2, \boldsymbol{X}'_1) \in \Sigma^{\text{fly}}$*, we have:*

$\text{supp}(\boldsymbol{X}'_4 \boldsymbol{X}'_3) \subseteq$ 

$\text{supp}(\boldsymbol{X}'_2 \boldsymbol{X}'_1) \subseteq$ 

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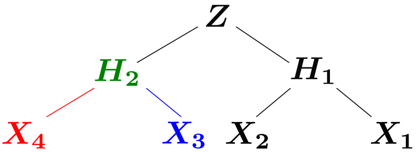

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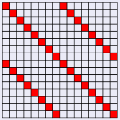
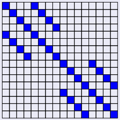
$\text{supp}(\boldsymbol{X}_4') \subseteq$ 

$\text{supp}(\boldsymbol{X}_3') \subseteq$ 

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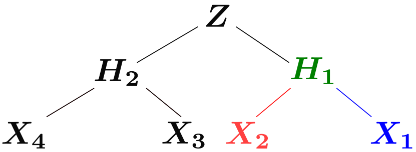

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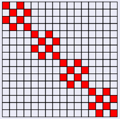
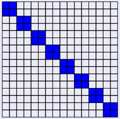
$\text{supp}(\mathbf{X}'_2) \subseteq$ 

$\text{supp}(\mathbf{X}'_1) \subseteq$ 

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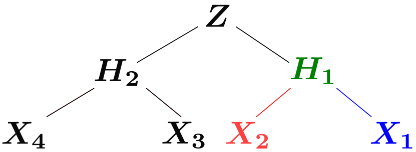

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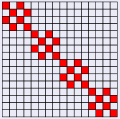
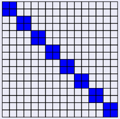
For any $(\boldsymbol{X}'_4, \boldsymbol{X}'_3, \boldsymbol{X}'_2, \boldsymbol{X}'_1) \in \Sigma^{\text{fly}}$, *we have:*

$\text{supp}(\boldsymbol{X}'_2) \subseteq$ 

$\text{supp}(\boldsymbol{X}'_1) \subseteq$ 

This property of the butterfly supports is true for any number of layers, and any hierarchical tree structure.

Exact recovery of the multiple butterfly factors

Let $\boldsymbol{Z} := \boldsymbol{X_L X_{L-1} ... X_1}$ of size $N = 2^L$ where supp($\boldsymbol{X_L}$), ..., supp($\boldsymbol{X_1}$) are exactly the butterfly supports.

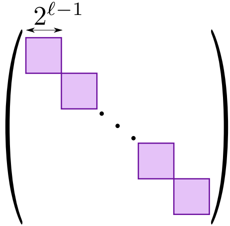
Algorithm Exact sparse recovery of $\boldsymbol{X_L}, ..., \boldsymbol{X_1}$ from $\boldsymbol{Z}$, up to rescaling.

Require: matrix $\boldsymbol{Z}$

$\boldsymbol{H} \leftarrow \boldsymbol{Z}$
for $\ell = L, ..., 1$ **do**
  $\mathcal{S} \leftarrow \varphi(\boldsymbol{B}^\ell, \boldsymbol{W}^{\ell-1})$
  for $i = 1, ..., r$ **do**
    $\boldsymbol{\mathcal{C}}^i \leftarrow \boldsymbol{H}_{|\boldsymbol{\mathcal{S}}^i}$
  end for
  $(\boldsymbol{X}'_\ell, \boldsymbol{H}^T) \leftarrow \varphi^{-1}(\mathcal{C})$
end for
return $\boldsymbol{X}'_L, ..., \boldsymbol{X}'_1$

$\boldsymbol{B}^\ell = \ell$-th butterfly support

$\boldsymbol{W}^{\ell-1} :=$



where  is a block full of 1s.

Recovery under noise: set $\boldsymbol{\mathcal{C}}^i$ as the best rank-one approximation of $\boldsymbol{H}_{|\boldsymbol{\mathcal{S}}^i}$.

Conclusion and discussion

Take-home message

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Future work

- Tighter conditions for fixed-support identifiability, to better understand identifiability of the support constraint.
- Identifiability in the multilayer case constrained by a *family* of sparsity patterns.

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