## Algorithmic and theoretical aspects of sparse deep neural networks

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## Deep learning and the recipe of success



Huge parametric models (over-parameterization)


Massive data set

High computing powers (GPUs)

## Deep learning and the recipe of success


? Can we make these three components scalable?

## Sparsity: a good old friend

## Sparse Deep Neural Networks



## Sparsity in Deep Neural Networks



## Questions for Sparse Neural Networks

```
Existence of optimal
    solutions
```

Tractability

Landscape

2 Does the training problem of sparse neural networks always admit an optimal solution?
? Is it polynomially tractable to train sparse neural networks?
? What does the landscape of loss function look like? (e.g., does it have local minima?, etc.)

Strategy:


## From sparsity in Deep Learning to Matrix Factorisation

## Sparse Matrix Factorisation

Given $A$ and $\mathscr{E}_{j}$ some sets of sparse matrices, solve:

$$
\min _{W^{(N)}, \ldots, W^{(1)}}\left\|A-\prod_{j=1}^{N} W^{(j)}\right\|_{F}^{2} \text { subject to: } W^{(j)} \in \mathscr{E}_{j}, \forall j \in\{1, \ldots, N\}
$$

- $k$-sparse per row,

- $k$-sparse in total

| Linear Sparse Neural Network | Sparse Matrix Factorisation |
| :--- | :--- |
| $\substack{\text { Minimize } \\ \mathbf{W}_{N}, \ldots, \mathbf{W}_{1}, \mathbf{b}}$ |  |

## Siparssupptrix faatroxifatitomization

Special case of sparse matrix factorization

SPARSE MATRIX FACTORISATION


## FIXED SUPPORT MATRIX FACTORISATION

$$
\min _{W^{(N)}, \ldots, W^{(1)}}\left\|A-\prod_{j=1}^{N} W^{(j)}\right\|_{F}^{2} \text { subject to: } W^{(j)} \in \mathscr{E}_{j}, \forall j \in\{1, \ldots, N\}
$$

$$
\cdot N=2
$$

- $\left(\mathscr{E}_{1}, \mathscr{E}_{2}\right)$ : set of matrices whose supports
are included in given sets $I$ and $J$ $\min _{X, Y}\left\|A-X Y^{\top}\right\|_{F}^{2}$ subject to: $\operatorname{supp}(X) \subseteq I, \operatorname{supp}(Y) \subseteq J$ $X, Y$


## Fixed support matrix factorization (FSMF)


$\mathrm{A} \approx$


SUPPORT CONTRAINTS
inside support
$\square$ outside support

## Overview of our reasoning



## Further motivation for sparse matrix factorization

Why sparse matrix factorisation?
Fast linear operator: if $\mathbf{A} \approx \mathbf{W}_{1} \ldots \mathbf{W}_{J}$ then $\mathbf{A x}=\mathbf{W}_{1} \ldots \mathbf{W}_{J} \mathbf{x}$

$O(n)$ nonzero entries

The Discrete Fourier Transformation sparse factorisation and its $O(n \log n)$ fast algorithm
Dictionary learning: given a dataset $\mathbf{Y}$, find atoms $\mathbf{D}$ and look-up table $\mathbf{X}$


## Plan of the talk




## Results on (FSMF)

## min <br> $X, Y$ <br> $L(X, Y)=\left\|A-X Y^{\top}\right\|_{F}^{2}$ subject to: $\operatorname{supp}(X) \subseteq I, \operatorname{supp}(Y) \subseteq J$

Existence of optimal solutions

Tractability

Landscape
[ Does (FSMF) always admit an optimal solution?

R Is (FSMF) polynomially tractable?
$\mathcal{B}$ What does the landscape of $L(X, Y)$ look like? (e.g., does it have local minima?, etc.)

## Non-existence of optimal solutions

## (FSMF) does not always admit an optimal solution



$$
\begin{aligned}
& A=\left(\begin{array}{ll}
0 & 1 \\
1 & 0
\end{array}\right) \\
& n=2
\end{aligned}
$$

亿 Infimum is zero: $X_{k}=\left(\begin{array}{cc}\frac{1}{k} & 0 \\ 1 & -1\end{array}\right), Y_{k}^{\top}=\left(\begin{array}{ll}1 & k \\ 0 & k\end{array}\right), \lim X_{k} Y_{k}^{\top}=A$. Unfimum is not attained: There is no feasible $(X, Y)$ such that $A=X Y^{\top}$.

## Equivalence between existence - closedness

ORIGINAL FORMULATION

EQUIVALENT FORMULATION

## $\min _{X Y}\left\|A-X Y^{\top}\right\|_{F}^{2}$ subject to: $\operatorname{supp}(X) \subseteq I, \operatorname{supp}(Y) \subseteq J$



$$
\min _{B \in \mathscr{P}_{I, J}}\|A-B\|_{F}^{2} \text { where } \mathscr{P}_{I, J}:=\left\{X Y^{\top} \mid \operatorname{supp}(X) \subseteq I, \operatorname{supp}(Y) \subseteq J\right\}
$$

PROJECTION OF $A$ ONTO THE SET $\mathscr{P}_{I, J}$

Optimal solutions exist if and only if $\mathscr{P}_{I, J}$ is closed

## Deciding the closedness of $\mathscr{P}_{I, J}$

Given $(I, J)$, decide the closedness of $\mathscr{P}_{I, J}$.
REMINDER: $\mathscr{P}_{I, J}:=\left\{X Y^{\top} \mid \operatorname{supp}(X) \subseteq I, \operatorname{supp}(Y) \subseteq J\right\}$


The emptyness of a semi-algebraic set is decidable (using Quantifier Elimination Algorithm).
(S. Basu, R. Pollack, M-F Roy, Algorithms in Real Algebraic Geometry)

U The complexity is doubly exponential (w.r.t. the sizes of $I, J$ and the matrix).

## NP-hardness

## THEOREM I

For arbitrary support constraint $(I, J)$, (FSMF) is NP-hard.

PROOF: Rank-one matrix completion is reducible to (FSMF).


## Tractability with structured supports

An example of tractable instances

## Unconstrained Matrix Factorisation

When there is no constraint on the supports of $(X, Y)$

$$
\underset{X \in \mathbb{R}^{n \times r}, Y \in \mathbb{R}^{m \times r}}{\operatorname{Minimize}} L(X, Y)=\left\|A-X Y^{\top}\right\|_{F}^{2}
$$



Best rank $r$ approximation of the matrix $A$.
\& Algorithm: Using (Truncated) Singular Value Decomposition.
? Can (Truncated) Singular Value Decomposition still work in constrained cases?

## Tractability with structured supports (cont)

Rank one contribution supports

$\square$ zeros

rank-one support

## Tractability with structured supports (cont)

## What is special about unconstrained matrix factorization?


!! All rank-one supports are identical

## THEOREM II

If all rank-one supports are pairwise disjoint or identical, then the corresponding instance of (FSMF) is polynomially tractable.

## Tractability with structured supports (cont)

## THEOREM II

If all rank-one supports are pairwise disjoint or identical, then the corresponding instance of (FSMF) is polynomially tractable.

ß Algorithm: Using (Truncated) Singular Value Decomposition for submatrices of the target matrix.

## Litteratures on the landscape of $L(X, Y)$

$$
L(X, Y)=\left\|A-X Y^{\top}\right\|_{F}^{2}
$$

Has been studied for:
Linear and shallow neural networks
凸 Matrix sensing, phase retrieval, matrix completion.
(Q. Li, Z. Zhu, G. Tang, The nonconvex geometry of low-rank matrix optimization, Information and Inference, 2018)
(Z. Zhu, D. Soudry, Y.C. Eldar, M.B. Wakin, The global optimization geometry of shallow linear neural networks, JMIV, 2019)
(L. Venturi, A. S. Bandeira, J. Bruna, Spurious valleys in one-hiddenlayer neural network optimization landscapes, JMLR, 2019)


What does the landscape look like in the constrained cases?

## Unconstrained matrix factorization

$$
L(X, Y)=\left\|A-X Y^{\top}\right\|_{F}^{2}
$$

$\Omega$ There is no spurious local minimum for any $A$.
$\Omega$ There is no spurious local valley for any $A$.

? Do these properties still hold in constrained cases?

## Benign landscape of tractable instances

## Reminder: Fixed Support Matrix Factorization

$$
\min _{X, Y}\left\|A-X Y^{\top}\right\|_{F}^{2} \text { subject to: } \operatorname{supp}(X) \subseteq I, \operatorname{supp}(Y) \subseteq J
$$

## THEOREM III

If $(I, J)$ satisfies the condition of Theorem II, then there is no spurious local minima and spurious local valleys.

## Summary on (FSMF)

## Existence of optimal solutions

-There are instances $(A, I, J)$ which (FSMF) admits no optimal solution.

NP-hardness $\quad \cdot$ For arbitrary $(I, J)$, (FSMF) is NP-hard to solve.
$\square$ -For certain structured $(I, J)$, (FSMF) has a polynomial algorithm.

Benign landscape
-With the same family of structured $(I, J)$, loss function of (FSMF) has no local minima.

[^0]
## Existence of optimal solutions in ReLU sparse neural network training



## Sparse ReLU Neural Networks Training

## Optimization problem of Sparse Neural Networks

Given data set $\mathscr{D}:=(X, Y)$ and $\mathscr{E}_{j}$ some sets of sparse matrices, solve:

$$
\begin{array}{ll}
\underset{W^{(j)}, b^{(j)}}{\operatorname{Minimize}} & \left\|Y-W^{(N)} \sigma\left(\ldots \sigma\left(W^{(1)} X+b^{(1)}\right)+\ldots\right)+b^{(N)}\right\|_{F}^{2} \\
\text { subject to: } & W^{(j)} \in \mathscr{E}_{j}, \forall j \in\{1, \ldots, N\}
\end{array}
$$

$\mathcal{\Omega}$ is the ReLU activation function: $\sigma(x)=\max (x, 0)$.
$\mathcal{G}$ In practice, $\mathscr{E}_{j}$ is usually chosen as the set of $\mathbf{k}$-sparse matrices.
(J. Frankle, M. Carbin, ICLR 2019), (S. Han, H. Mao, W-J. Dally, ICLR 2016)
$\}$ We consider quadratic loss function for simplification. Our argument works for any coercive loss function.

## Non-existence of optimal solutions - ill-posedness


$\left.\begin{array}{|c|c|}\hline \text { Tensor decomposition } \\ \text { (order at least three) }\end{array} \begin{array}{c}\text { TENSOR RANK AND THE LLL-POSEDNESS OF THE BEST } \\ \text { LOW-RANK APPROXIMATION PROBLEM } \\ \text { VIN DE SLVA* AND LEK-HENG Lim }\end{array}\right\}$

How about the training problem of sparse ReLU neural networks?

## Fixed support sparse ReLU neural networks

Given data set $\mathscr{D}:=(X, Y)$, solve:


## DÉJÀ VU: closedness vs existence of optimal solutions



The support constraint $\left(I_{1}, \ldots, I_{N}\right)$ makes the training problem always admit optimal solutions if and only if for all input sets $X$, the image of the function $\theta:=\left\{\left(W^{i}, b^{i}\right)\right\} \mapsto W^{(N)} \sigma\left(\ldots \sigma\left(W^{(1)} X+b^{(1)}\right)+\ldots\right)+b^{(N)}$
 is closed.

## Sufficient condition for the existence of optimal solutions

## THEOREM IV

For two-layer neural networks ( $N=2$ ) with output dimension equal to one, any support constraint makes the training problem always admit optimal solutions.
(Q-T. Le, E. Riccietti, R. Gribonval, preprint, 2023)

## COROLLARY I

For two-layer neural networks $(N=2)$ with output dimension equal to one, the constraints $\mathscr{E}_{j}:=\left\{X \mid\|X\|_{0} \leq k_{j}\right\}, j=1,2$ makes the training problem always admit optimal solutions.

## Necessary condition for the existence of optimal solutions

## THEOREM V

For two-layer neural networks $(N=2)$ with support constraint $(I, J)$, if the training problem always admits optimal solutions, then $\mathscr{P}_{I, J}$ is closed.
(Q-T. Le, E. Riccietti, R. Gribonval, preprint, 2023)

$$
\mathscr{P}_{I, J}:=\left\{X Y^{\top} \mid \operatorname{supp}(X) \subseteq I, \operatorname{supp}(Y) \subseteq\right. \text { 场js is decidable }
$$

## THEOREM VI

For fixed support neural networks with support constraint $/\left(I_{1}, \ldots, I_{N}\right)$, if the training problem always admits optimal solutions, then $\mathscr{P}_{I_{1}, \ldots, I_{N}}$ is closed.

## Necessary condition for the existence of optimal solutions

## THEOREM

For two-layer neural networks $(N=2)$ with support constraint $(I, J)$, if the training problem always admits optimal solutions, then $\mathscr{P}_{I, J}$ is closed.

The condition is just necessary because when there is no constraint on the support, the training problem is ill-posed for certain data set.

## Butterfly

 parameterization in sparse neural networks
## Introduction to butterfly parameterization

Discrete Fourier Transform (DFT): $\quad y_{k}=\sum_{n=0}^{N-1} e^{-\frac{i \pi}{N} k n} x_{n}, \quad k=0, \ldots, N-1$

$$
y=F_{N} x \quad F_{N}=\left(e^{-\frac{i 2 \pi}{N} k n}\right)_{k, n \in\{0, \ldots, N-1\}}
$$

Algebraic properties of the Fourier kernel:

$$
y_{k}=\sum_{m=0}^{N / 2-1} e^{-\frac{i 2 \pi}{N / 2} k m} x_{2 m}+e^{-\frac{i 2 \pi}{N} k} \sum_{m=0}^{N / 2-1} e^{-\frac{i 2 \pi}{N / 2} k m} x_{2 m+1} e^{-\frac{i 2 \pi}{N / 2} k m} x_{2 m}-e^{-\frac{i 2 \pi}{N} k} \sum_{m=0}^{N / 2-1} e^{-\frac{i 2 \pi}{N / 2} k m} x_{2 m+1} \quad \begin{aligned}
& \text { The Cooley - Tukey } \\
& \text { algorithm (radix-2) }
\end{aligned}
$$

## Matrix factorization of DFT

$$
\begin{aligned}
& F_{N} x=\binom{F_{N / 2} x_{e}+D_{N / 2} F_{N / 2} x_{o}}{F_{N / 2} x_{e}-D_{N / 2} F_{N / 2} x_{o}} \\
& =\left(\begin{array}{ll}
I_{N / 2} & D_{N / 2} \\
I_{N / 2} & -D_{N / 2}
\end{array}\right)\left(\begin{array}{cl}
F_{N / 2} & 0 \\
0 & F_{N / 2}
\end{array}\right) P_{N} x \\
& D_{N 2}=\int^{1} \begin{array}{ll} 
& \\
& e^{-\frac{i v \pi}{N}}
\end{array} \\
& \text { Unrolling the recursion: } \\
& \text { Permutation matrix }
\end{aligned}
$$

$$
\begin{aligned}
F_{N} & =B_{N}\left(\begin{array}{rl}
F_{N / 2} & \mathbf{0} \\
\mathbf{0} & F_{N / 2}
\end{array}\right) P_{N} \\
& =B_{N}\left(\begin{array}{rl}
B_{N / 2} & \mathbf{0} \\
\mathbf{0} & B_{N / 2}
\end{array}\right)\left(\begin{array}{llll}
B_{N / 4} & & & \\
& B_{N / 4} & & \\
& & B_{N / 4} & \\
& & & B_{N / 4}
\end{array}\right)\left(\begin{array}{cc}
P_{N / 2} & \mathbf{0} \\
\mathbf{0} & P_{N / 2}
\end{array}\right) P_{N} \\
& =\ldots
\end{aligned}
$$

## Matrix factorization of DFT



## Butterfly parameterization in Sparse Neural Networks

Classical neural networks

## $x+b$ <br> $O\left(N^{2}\right)$


$\longrightarrow$

Butterfly sparse neural networks


| Parameterization | Number of factors | Matrix size | Introduced by |
| :---: | :---: | :---: | :---: |
| Butterfly | L | $2^{L} \times 2^{L}$ | T. Dao et. al., 2019 |
| Kaleidoscope | 2 L | $2^{L} \times 2^{L}$ | T. Dao et. al., 2020 |
| Monarch | 2 | $m \times n$ | T. Dao et. al., 2022 |
| Deformable butterfly | flexible | $m \times n$ | R. Lin et. al., 2022 |

. Supports of factors are fixed, sparse and very structured.

## Interpretation of butterfly parameterization

? Among all existing parameterization, which one should we choose?


Trade-off between performance and compression

## Approximation a matrix by butterfly parameterization

$$
\min _{W^{(1)}, \ldots, W^{(L)}}\left\|A-W^{(1)} \ldots W^{(L)}\right\|_{F} \quad \text { s.t. } W^{(t)} \text { is butterfly }
$$

\& Generalized version of (FSMF) with structured supports.
E Existing algorithm: hierarchical factorization - butterfly algorithm.
(Michielssen \& Boag, 1996); (O'Neil, Woolfe \& Rokhlin, 2010); (Liu et. al. 2021)
No theoretical guarantee yet.
!. Hypothesis class of matrix:

$$
\mathscr{B}:=\left\{W^{(1)} \ldots W^{(L)} \mid \text { Infimum of }(1)=0\right\}
$$

## Analysis of butterfly parameterization

## THEOREM VII

If $E^{*}$ is the best error approximation of (1), the butterfly algorithm yields a solution whose distance to $A$ is smaller than $\left(2^{L-1}-1\right) E^{*}$

Algebraic description of $\mathscr{B}$ :

$\Omega$ Also known as complementary low-rank matrices in the literature.

## Contribution and future works

## TAKE AWAY MESSAGE

- Link between sparse matrix factorization and its variant (FSMF) with sparse ReLU neural networks.
- Necessary/Sufficient condition for the existence of optimal solutions sparse ReLU neural networks.
-Butterfly parameterization in sparse deep neural networks


## POSSIBLE IMPROVEMENT?

- Better algorithms to decide the ill-posedness of (FSMF).
- A full characterization of ill-posedness of sparse ReLU neural networks.
https://faust.inria.fr/
https://arxiv.org/abs/2112.00386 https://arxiv.org/abs/2306.02666


## THANK YOU

## Analysis of butterfly parameterization

- The supports of all existing factors have the form:

$$
\operatorname{supp}\left(W^{(\ell)}\right) \subseteq \mathbf{I}_{a} \otimes \mathbf{1}_{b \times c} \otimes \mathbf{I}_{d}
$$

EXAMPLE:

| Parameterization | Support forms |
| :---: | :---: |
| Butterfly | $\mathbf{I}_{2^{\ell-1}} \otimes \mathbf{1}_{2 \times 2} \otimes \mathbf{I}_{\frac{N}{2 \epsilon}}$ |
| Kaleidoscope | $\mathbf{1}_{a \times b} \otimes \mathbf{I}_{c}$ and $\mathbf{I}_{b} \otimes \mathbf{1}_{c \times d}$ |
| Monarch | $\mathbf{I}_{a} \otimes \mathbf{1}_{b \times c} \otimes \mathbf{I}_{d}$ |
| Deformable butterfly |  |

- The product of two consecutive factors remains butterfly .

$$
\operatorname{supp}\left(W^{(\ell)} W^{(\ell+1)}\right) \subseteq \mathbf{I}_{a^{\prime}} \otimes \mathbf{1}_{b^{\prime} \times c^{\prime}} \otimes \mathbf{I}_{d^{\prime}}
$$

\ This does not include the Kaleidoscope parameterization.

## And Fixed Support Matrix Factorization

$A=$

$X$


LU decomposition


Low rank approximation

(b) $\mathbf{S}_{\mathrm{bf}}^{(3)}$

Butterfly matrix factorization
(d) $\mathbf{S}_{\mathrm{bf}}^{(1)}$

(c) $\mathbf{S}_{\mathrm{bf}}^{(2)}$


(a) $\mathbf{S}_{\mathrm{bf}}^{(4)}$
(a) $\mathrm{S}_{\mathrm{bf}}$


Hierarchical matrix

## Question for sparse neural networks

## Problem formulation

Feed forward networks:

$$
\begin{gathered}
\theta=\left\{\left(\mathbf{W}_{i}, \mathbf{b}_{i}\right) \mid i=1, \ldots, N\right\} \\
f(x ; \theta)=\mathbf{W}_{N} \sigma\left(\ldots \sigma\left(\mathbf{W}_{1} x+\mathbf{b}_{1}\right)\right)+\mathbf{b}_{N}
\end{gathered}
$$

Training:

| Conventional Deep Neural Networks |  | Sparse Deep Neural Networks |  |
| :---: | :---: | :---: | :---: |
| $\underset{\theta}{\text { Minimize: }} \quad \mathscr{L}_{\theta}:=\sum_{i=1}^{n} L\left(f\left(\theta, x_{i}\right), y_{i}\right)$ | Minimize: <br> such that: | $\mathscr{L}_{\theta}:=\sum_{i=1}^{n} L\left(f\left(\theta, x_{i}\right), y_{i}\right)$ |  |
| $\mathbf{W}_{i}$ are sparse matrices |  |  |  |

Existing algorithms / approaches for Sparse Deep Neural Networks training:
-Pruning \& Retraining, Lottery Ticket Hypothesis (Han et al., IPL 2015), (Zhu et al., 2017), (Jonathan et al., 2019) -Regularisation $l_{0}$ or $l_{1}$
-Bayesian/ Variational approaches
(Bengio et al., 2013), (Yu et al., 2017), (Collins et al., 2014), (Liu et al., 2015)
( Neklyudov et al., 2017), (Ullrich et al., 2017), (Louizos et al., 2017)


[^0]:    (Q-T. Le, E. Riccietti, R. Gribonval, SIAM Journal of Matrix Analysis and Applications, 2023)

