



Algorithmic and theoretical aspects of sparse deep neural networks

Quoc Tung Le

lazia

July 26th, 2023









Elisa Riccietti



Rémi Gribonval

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





Sounds good. Then how can I train a sparse neural network?





Linear

Nonlinear

Activation function







Questions for Sparse Neural Networks

Existence of optimal solutions

Tractability

Landscape

neural networks?

Strategy:



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





From sparsity in Deep Learning to Matrix Factorisation

Sparse Matrix Factorisation

Given A and \mathscr{E}_i some sets of **sparse** matrices, solve: $\min_{W^{(N)},...,W^{(1)}} \|A - \prod_{j=1}^{N} W^{(j)}\|_{F}^{2} \text{ subject to: } W^{(j)} \in \mathscr{C}_{j}, \forall j \in \{1,...,N\}$

Linear Sparse Neural Network

 $\|\mathbf{Y} - \mathbf{W}_N \dots \mathbf{W}_1 \mathbf{X} - \mathbf{b}\|_F^2$ Minimize $W_N,...,W_1,b$

- - k-sparse per row,
- Choic of spaine an appages Set Gal Network parse page Collatin Factorisation
 - k-sparse in total

Sparse Matrix Factorisation

 $\|\mathbf{A} - \mathbf{W}_N \dots \mathbf{W}_1\|_F^2$ Minimize $\mathbf{W}_N,\ldots,\mathbf{W}_1$



Special case of sparse matrix factorization

SPARSE MATRIX FACTORISATION





FIXED SUPPORT MATRIX FACTORISATION

X, Y

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

 $\cdot N = 2$ • $(\mathscr{E}_1, \mathscr{E}_2)$: set of matrices whose supports are included in given sets I and J

min $||A - XY^{\top}||_F^2$ subject to: supp $(X) \subseteq I$, supp $(Y) \subseteq J$

Fixed support matrix factorization (FSMF)

Х

X, Y





inside support





SUPPORT CONTRAINTS

outside support

Overview of our reasoning



Sparse Matrix Factorization

Existence of optimal solutions

Tractability

Landscape



Linear activation + No bias

Sparse Deep Neural Networks

Existence of optimal solutions

Tractability

Landscape

Further motivation for sparse matrix factorization

Why sparse matrix factorisation?

Fast linear operator: if $\mathbf{A} \approx \mathbf{W}_1 \dots \mathbf{W}_J$ then $\mathbf{A}\mathbf{x} = \mathbf{W}_1 \dots \mathbf{W}_J \mathbf{x}$



The Discrete Fourier Transformation sparse factorisation and its $O(n \log n)$ fast algorithm

Dictionary learning: given a dataset **Y**, find atoms **D** and look-up table **X**



log *n* factors

Plan of the talk

Existence of optimal solutions in sparse ReLU neural networks training

Fixed Support Matrix Factorisation

Butterfly parameterization in sparse deep neural networks



Fixed support matrix factorization



Results on (FSMF)

min $L(X, Y) = ||A - XY^{\top}||_F^2$ subject to: supp $(X) \subseteq I$, supp $(Y) \subseteq J$ X.Y

Existence of optimal solutions

Tractability

Landscape

 $\int \mathcal{P}$ Does (FSMF) always admit an optimal solution?

- Solution of the second second
- \mathcal{D} What does the **landscape** of L(X, Y) look like? (e.g., does it have **local minima**?, etc.)

Existence of optimal solutions

Non-existence of optimal solutions



$$A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$
$$n = 2$$

 $\int \mathcal{T}$ Infimum is **not** attained: There is no feasible (X, Y) such that $A = XY^{\top}$. (Gene H. Golub and Charles F. Van Loan, Matrix Computations)

(FSMF) does not always admit an optimal solution



Existence of optimal solutions

Equivalence between existence - closedness

ORIGINAL FORMULATION



EQUIVALENT FORMULATION

X.Y

 $B \in \mathcal{P}_{II}$



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



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

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

Existence of optimal solutions

Deciding the closedness of \mathcal{P}_{IJ}

Given (I, J), decide the **closedness** of $\mathscr{P}_{I,J}$.

 $\mathscr{P}_{I,J}$ is closed?

Elimination Algorithm).

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

REMINDER: $\mathscr{P}_{I,J} := \{XY^{\top} \mid \operatorname{supp}(X) \subseteq I, \operatorname{supp}(Y) \subseteq J\}$

is empty

(S. Basu, R. Pollack, M-F Roy, Algorithms in Real Algebraic Geometry)

set

NP-hardness

THEOREM I

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

					\wedge			
2	?	1	?	?				
?	2	?	4	0				
?	9	?	?	1				
5	?	2	9	?				

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

This problem is NP-hard.

(N.Gillis, F. Glineur, SIAM Journal on Matrix Analysis and Applications)

Tractability with structured supports

An example of tractable instances

Unconstrained Matrix Factorisation

 $X \in \mathbb{R}^{n \times r}, Y \in \mathbb{R}^{m \times r}$

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

CP Algorithm: Using (Truncated) Singular Value Decomposition. Can (Truncated) Singular Value Decomposition still work in constrained cases?

Minimize $L(X, Y) = ||A - XY^{\top}||_F^2$

Best rank r approximation of the matrix A.

(S. Burer, R. D.C. Monteiro, Mathematical Programming)

Tractability with structured supports (cont)

Rank one contribution supports

kth column of X

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

corresponding instance of (FSMF) is polynomially tractable.

rank-one supports

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

If all rank-one supports are pairwise disjoint or identical, then the

Litteratures on the landscape of L(X, Y)

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

Has been studied for:

Linear and shallow neural networks

$\int \mathcal{P}$ 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)

Landscape

Unconstrained matrix factorization

 $\int \mathcal{T}$ There is no spurious local minimum for any A. $\int \mathcal{T}$ There is no spurious local valley for any A.

Do these properties still hold in constrained cases?

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

Landscape

Benign landscape of tractable instances

Reminder: Fixed Support Matrix Factorization

X, Y

THEOREM III

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

min $||A - XY^{\top}||_F^2$ subject to: supp $(X) \subseteq I$, supp $(Y) \subseteq J$

Summary on (FSMF)

Existence of optimal solutions	 There are instance optimal solution.
NP-hardness	•For arbitrary (I, J)
Tractability	 For certain structual algorithm.
Benign landscape	•With the same far

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

es (A, I, J) which (FSMF) admits no

(), (FSMF) is NP-hard to solve.

ured (I, J), (FSMF) has a polynomial

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

Existence of optimal solutions in ReLU sparse neural network training

Sparse ReLU Neural Networks Training

Optimization problem of Sparse Neural Networks

Minimize $W^{(j)}.b^{(j)}$ subject to: $W^{(j)} \in \mathscr{E}_i$,

 $\int \sigma$ is the **ReLU** activation function: $\sigma(x) = \max(x,0)$.

 $\int \mathcal{P}$ In practice, \mathscr{E}_i is usually chosen as the set of **k-sparse matrices**.

 $\int \mathcal{P}$ We consider quadratic loss function for simplification. Our argument works for any **coercive** loss function.

Given data set $\mathscr{D} := (X, Y)$ and \mathscr{C}_i some sets of **sparse** matrices, solve: $\|Y - W^{(N)}\sigma(\dots\sigma(W^{(1)}X + b^{(1)}) + \dots) + b^{(N)}\|_{F}^{2}$

$$\forall j \in \{1, \dots, N\}$$

(J. Frankle, M. Carbin, ICLR 2019), (S. Han, H. Mao, W-J. Dally, ICLR 2016)

Non-existence of optimal solutions - ill-posedness

Tensor decom (order at least

Matrix Comp

Robust Prin Component A

> (Classical) N **Network Tra**

How about the training problem of sparse ReLU neural networks?

position t three)	TENSOR RANK AND THE ILL-POSEDNESS OF THE BEST LOW-RANK APPROXIMATION PROBLEM VIN DE SILVA [*] AND LEK-HENG LIM [†]		
oletion	Low-Rank Matrix Approximation with Weights or Missing Data is NP-hard ^{Nicolas Gillis¹} and François Glineur ¹		
nciple Analysis	Matrix rigidity and the ill-posedness of Robust PCA and matrix completion [*] Jared Tanner ^{†‡} Andrew Thompson [§] Simon Vary [†]		
Veural aining	Best <i>k</i>-Layer Neural Network Approximations Lek-Heng Lim ¹ · Mateusz Michałek ^{2,3} · Yang Qi ⁴		

Fixed support sparse ReLU neural networks

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

GENERAL

FIXED SUPPORT

$$Y - W^{(L)}\sigma(\dots\sigma(W^{(1)}X + b^{(1)}) + \dots) + b^{(L)}\|_F^2$$
$$V^{(j)} \in \mathcal{C}_j, \forall j \in \{1, \dots, N\}$$

$$Y - W^{(N)}\sigma(\dots\sigma(W^{(1)}X + b^{(1)}) + \dots) + b^{(N)}\|_{F}^{2}$$
$$upp(W^{(j)}) \in I_{j}, \forall j \in \{1,\dots,N\}$$

DÉJÀ VU: closedness vs existence of optimal solutions

The support constraint (I_1, \ldots, I_N) makes the training problem **always** admit optimal solutions if and only if for all input sets X, the image of the function $\theta := \{ (W^i, b^i) \} \mapsto W^{(N)} \sigma(...\sigma(W^{(1)}X + b^{(1)}) + ...) + b^{(N)} \}$ is closed.

Given a support constraint (I_1, \ldots, I_N) , does optimal solutions always exist for all data set \mathcal{D} for the corresponding training problem ?

Sufficient condition for the existence of optimal solutions

THEOREM IV

(Q-T. Le, E. Riccietti, R. Gribonval, preprint, 2023)

COROLLARY

admit optimal solutions.

For two-layer neural networks (N = 2) with output dimension equal to one, any support constraint makes the training problem always admit optimal solutions.

For two-layer neural networks (N = 2) with output dimension equal to one, the constraints $\mathscr{C}_i := \{X \mid ||X||_0 \le k_i\}, j = 1, 2$ makes the training problem **always**

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}_{IJ} is closed.

(Q-T. Le, E. Riccietti, R. Gribonval, preprint, 2023)

$$\mathscr{P}_{I,J} := \{ XY^{\mathsf{T}} \mid \mathsf{supp}(X) \}$$

THEOREM VI

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.

(L-H. Lim, M. Michalek, Y. Qi, Constructive Approximation 2019)

Butterfly parameterization in sparse neural networks

Introduction to butte

Discrete Fourier Transform (DFT): y_k

y

Algebraic properties of the Fourier kernel:

$$y_{k} = \sum_{\substack{m=0\\N/2-1\\N/2-1}}^{N/2-1} e^{-\frac{i2\pi}{N/2}km} x_{2m} + e^{-\frac{i2\pi}{N/2}km} x_{2m} - e^{-\frac{i2\pi}{N/2}km$$

DFT on **even** indices

rfly parameterization
=
$$\sum_{n=0}^{N-1} e^{-\frac{i2\pi}{N}kn} x_n$$
, $k = 0, ..., N-1$
= $F_N x$ $F_N = \left(e^{-\frac{i2\pi}{N}kn}\right)_{k,n \in \{0,...,N-1\}}$

37

The Cooley - Tukey algorithm (radix-2)

DFT on **odd** indices

Matrix factorization of DFT

$$F_{N}x = \begin{pmatrix} F_{N/2}x_{e} + D_{N/2}F_{N/2}x_{o} \\ F_{N/2}x_{e} - D_{N/2}F_{N/2}x_{o} \end{pmatrix}$$
$$= \begin{pmatrix} I_{N/2} & D_{N/2} \\ I_{N/2} & -D_{N/2} \end{pmatrix} \begin{pmatrix} F_{N/2} & \mathbf{0} \\ \mathbf{0} & F_{N/2} \end{pmatrix} \boxed{P_{N}x}$$

Unrolling the recursion:

$$F_{N} = B_{N} \begin{pmatrix} F_{N/2} & \mathbf{0} \\ \mathbf{0} & F_{N/2} \end{pmatrix} P_{N}$$
$$= B_{N} \begin{pmatrix} B_{N/2} & \mathbf{0} \\ \mathbf{0} & B_{N/2} \end{pmatrix} \begin{pmatrix} B_{N/2} & \mathbf{0} \\ \mathbf{0} & B_{N/2} \end{pmatrix}$$
$$= \dots$$

Matrix factorization of DFT

Assume that $N = 2^L$:

For N = 16:

Classical neural networks

$$x + b$$

 $O(N^2)$

Parameterization	Number of factors	Matrix size	Introduced by	
Butterfly		$2^L \times 2^L$	T. Dao et. al., 2019	
Kaleidoscope	2L	$2^L \times 2^L$	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

$$\min_{W^{(1)},\ldots,W^{(L)}} \|A - W^{(1)} \ldots W^{(L)}\|_F$$

Generalized version of (FSMF) with structured supports. $\int \mathcal{P}$ 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:

s.t. $W^{(\ell)}$ is butterfly

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

Analysis of butterfly parameterization

THEOREM VII

a solution whose distance to A is smaller than $(2^{L-1} - 1)E^*$

Algebraic description of \mathscr{B} :

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

If E^* is the best error approximation of (1), the butterfly algorithm yields

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.

THANK YOU

https://faust.inria.fr/ https://arxiv.org/abs/2112.00386 https://arxiv.org/abs/2306.02666

Analysis of butterfly parameterization

The supports of all existing factors have the form:

EXAMPLE:

Parameterization

Butterfly

Kaleidoscope

Monarch

Deformable butterfly

The product of two consecutive factors remains butterfly. $supp(W^{(\ell)}W^{(\ell)})$

This does not include the Kaleidoscope parameterization.

$$\subseteq \mathbf{I}_a \otimes \mathbf{1}_{b \times c} \otimes \mathbf{I}_d$$

Support forms
 $\mathbf{I}_{2^{\ell-1}} \otimes 1_{2 \times 2} \otimes \mathbf{I}_{\frac{N}{2^{\ell}}}$
$1_{a \times b} \otimes \mathbf{I}_{c}$ and $\mathbf{I}_{b} \otimes 1_{c \times d}$
$\mathbf{I}_a \otimes 1_{b \times c} \otimes \mathbf{I}_d$

$$^{(+1)}) \subseteq \mathbf{I}_{a'} \otimes \mathbf{1}_{b' \times c'} \otimes \mathbf{I}_{d'}$$

LU decomposition

Low rank approximation

Butterfly matrix factorization

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 (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)

- •Bayesian/ Variational approaches

 $\theta = \{ (\mathbf{W}_i, \mathbf{b}_i) \mid i = 1, ..., N \}$ $f(x; \theta) = \mathbf{W}_N \sigma(\dots \sigma(\mathbf{W}_1 x + \mathbf{b}_1)) + \mathbf{b}_N$

Sparse Deep Neural Networks				
$\underset{\theta}{Minimize:}$	$\mathscr{L}_{\theta} := \sum_{i=1}^{n} L(f(\theta, x_i), y_i)$			
such that:	\mathbf{W}_i are sparse matrices			

