Sparse Matrix Factorization from an Optimization Point of View

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Sparse matrix factorization

Objective: Given A, find *multiple* factors $S^{(1)}, S^{(2)}, \ldots, S^{(J)}$ such that:

$$A \approx S^{(1)} S^{(2)} \ldots S^{(J)}$$

where $S^{(i)}$ are *sparse* matrices.

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Motivations

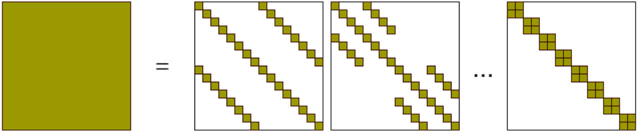
- *Fast* matrix vector products:

$$\underbrace{A}_{\textit{dense}} \approx \underbrace{S^{(1)} S^{(2)} \ldots S^{(J)}}_{\textit{sparse}} \quad \Rightarrow \quad Ax \approx S^{(1)}(S^{(2)}(\ldots(S^{(J)}x)))$$

- Reduce time + memory complexity

Applications

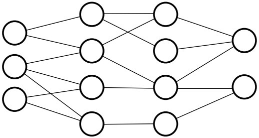
- **Fast Fourier Transform**, **Fast Hadamard Transform**, etc.



- **Dictionary learning**
  - $A = XY^\top$, A data, X a base (words in a dictionary), Y representation of each sample using the dictionary.

[S. Foucart, H. Rauhut, **A mathematical introduction to compressive sensing**, ANHA, 2013]

- **Sparse (linear) neural networks**:
  - Interpretability.
  - Energy efficiency.



[T. Dao & all. **Learning fast algorithms for linear transforms using butterfly factorizations**, PMLR, 2019]
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A general formulation for sparse matrix factorization

Sparse Matrix Factorization Problem

Given A and $\mathcal{E}_j$ some sets of sparse matrices, solve:

$$\min_{S^{(1)},\ldots,S^{(J)}} \|A - \prod_{j=1}^{J} S^{(j)}\|_F^2 \quad \text{subject to:} \quad S^{(j)} \in \mathcal{E}_j, \forall j \in \{1, \ldots, J\}$$

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- Example of *sparsity patterns* $\mathcal{E}_j$: set of matrices with at most k nonzero entries per row, per column or in total.
- Known to be **NP-hard** (covers sparse PCA, sparse dictionary learning)

  [Malik, **NP-hardness and inapproximability of sparse PCA**, IPL, 2017]
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→ A challenging problem, how to deal with it?

Our approach: from two to multiple factors

- **Two** factors matrix factorization: the simplest nontrivial case.

$$\text{Given } A, \underset{X,Y}{\text{minimize}} \|A - XY^\top\|_F^2 \text{ subject to: } X, Y \text{ sparse matrices}$$

- **Multiple** factors matrix factorization: butterfly factorization.

Two sub-problems of **two** factors matrix factorization

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Find *two* sets S_X, S_Y - the supports of two factors X, Y

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$$\underset{X \in \mathbb{R}^{m\times r}, Y \in \mathbb{R}^{n \times r}}{\text{Minimize}} \quad L(X, Y) = \|A - XY^\top\|_F^2$$

Subject to: $\quad \mathrm{supp}(X) \subseteq S_X$

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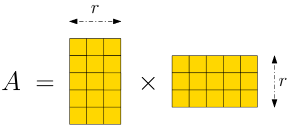
$\rightarrow$ Second problem: Fixed support matrix factorization (FSMF).

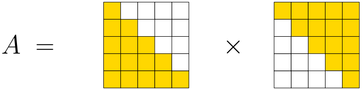
Examples of FSMF

FSMF covers:

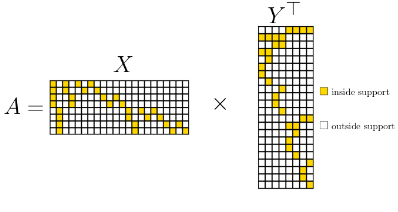
- Low rank matrix decomposition



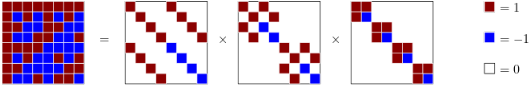
- LU decomposition



- Hierarchical $\mathcal{H}$ matrices

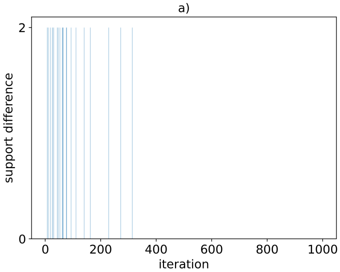


- Butterfly factorization (multiple factors)



Understand the *asymptotic behaviour* of other existing heuristics:

- Supports asymptotically don't change
- Spurious local valley in the landscape of $L(X, Y)$: certain heuristic can lead to iterates diverging to infinity



Measure of the difference between two consecutive supports

[L. Le Magoarou and R. Gribonval, **Chasing butterflies: In search of efficient dictionaries**, ICASSP, 2015]

Main contributions on FSMF

1. Is the problem polynomially tractable?
   → We prove its *NP-hardness*.

2. Does the problem have a solution?
   → We show an instance where optimal solutions do *not* exist.

3. Are there easy instances?
   → We individuate a family of *polynomially solvable* instances and proposed an *efficient algorithm*.

4. How well does gradient descent tackle the problem of FSMF?
   → We study the properties of the *landscape* of the function $L(X, Y) = \|A - XY^\top\|^2$ *under the support constraints*.

NP-hardness

Theorem (1)

Sparse matrix factorization is NP-hard even with fixed support

Proof.

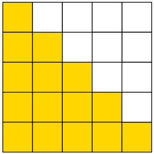
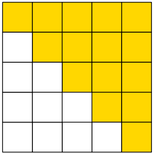
Rank-one matrix completion with noise is reducible to FSMF. □

- In line with recent results on matrix factorization:
  - non-negative matrix factorization (NMF)
  - weighted low rank
  - matrix completion

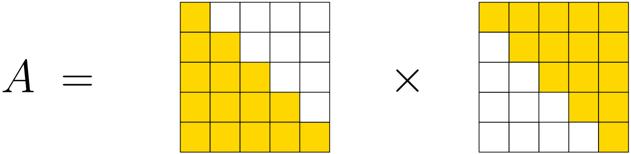
[N. Gillis, F. Glineur, Low-rank matrix approximation with weights or missing data is NP-hard. SIAM JMAA, 2010]

[S. A. Vavasis, On the complexity of nonnegative matrix factorization, SIOPT, 2010]

LU decomposition and non-closedness

$A =$  $\times$ 

LU decomposition and non-closedness



- Fact: Any square matrix is the limit of a sequence of matrices having an LU decomposition.
- But there exist square matrices that **do not have** an exact LU decomposition.

[H. Golub and C. F. Van Loan, **Matrix Computations**, **The Johns Hopkins University Press**]

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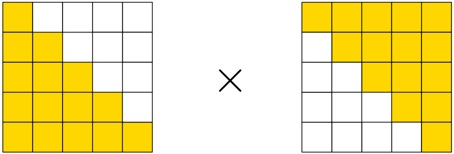

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$\longrightarrow$ The set of matrices having LU decomposition is not closed
$\longrightarrow$ For certain support constraints (S_X, S_Y) and matrices A, (FSMF) does not have an optimal solution.

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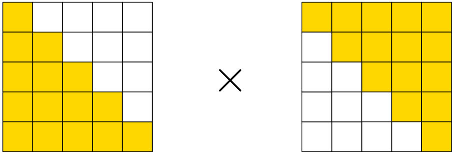
$A =$ 

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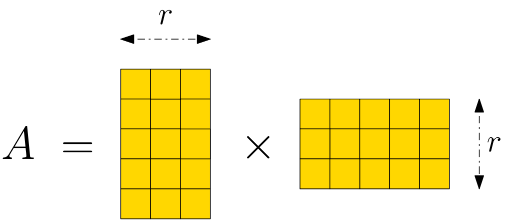
$\longrightarrow$ For certain support constraints (S_X, S_Y) and matrices A, (FSMF) does not have an optimal solution.
Question : Given (S_X, S_Y), do their FSMF instances always have optimal solutions? $\rightarrow$ This problem is *decidable* (not known to be *tractable* yet).

Polynomially solvable instances

Example (Unconstrained matrix factorization)

When there is no constraints on the support of X and Y:

$$\underset{X \in \mathbb{R}^{m \times r}, Y \in \mathbb{R}^{n \times r}}{\text{Minimize}} \; L(X, Y) = \|A - XY^\top\|_F^2$$



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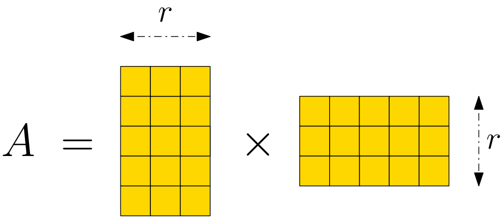

→ Solution: Use Singular Value Decomposition (SVD).

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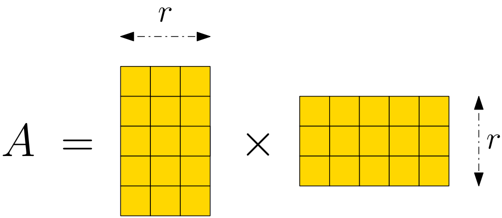

→ Solution: Use Singular Value Decomposition (SVD).

→ Question: Can Singular Value Decomposition (SVD) still work in the *constrained* case?

SVD as a greedy algorithm

1) Decompose the problem:

$$A - XY^\top = A - \sum_{i=1}^{r} x_i y_i^\top = A - \sum_{i=1}^{r} \underbrace{M_i}_{\text{rank-one}} \quad (M_i := x_i y_i^\top)$$

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2) Finding the SVD:

$$\begin{aligned}
&\texttt{bestRankOneApprox}(A) && \to M_1 \\
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&\dots && \\
&\texttt{bestRankOneApprox}(A - M_1 \dots - M_{r-1}) && \to M_r
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$\to$ SVD is a greedy algorithm in disguise

Algorithm 1 Algorithm for *unconstrained* matrix factorization

1: **for** $i \in \{1, \dots, r\}$ **do**
2: $M_i :=$ best rank-one approximation of $A - \sum_{k=1}^{i-1} M_k$.
3: **end for**

SVD as a greedy algorithm: the *constrained* case

- How to generalize the greedy algorithm?

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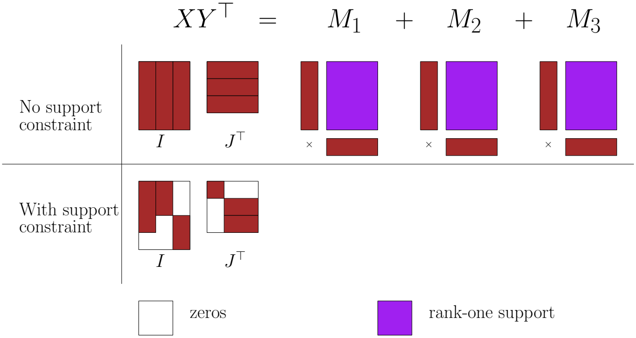

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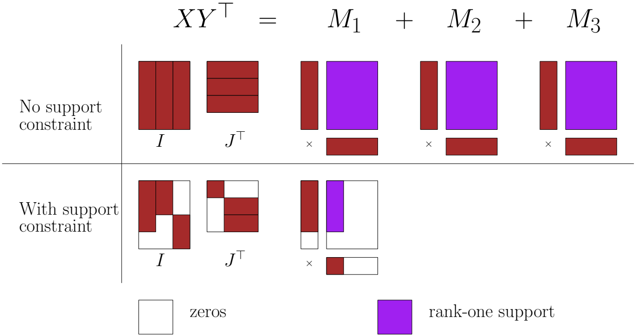

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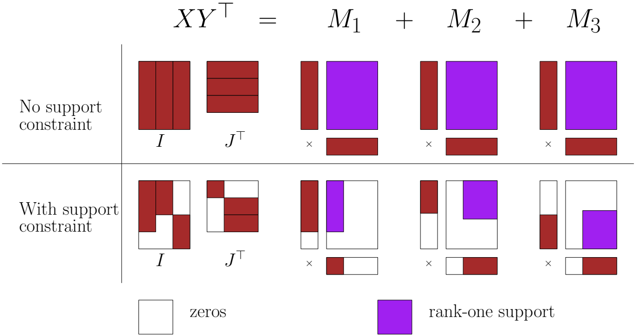
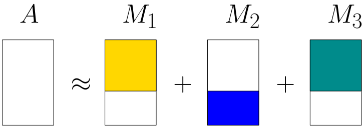


- Finding optimal solution (X, Y) $\rightleftarrows$ Finding optimal the rank-one constrained supports.

Algorithm 2 Algorithm for fixed-support matrix factorization

for $i \in \{1, \dots, r\}$ **do**
  $S_i \leftarrow i$-th rank-one support
  $M_i :=$ best rank-one approximation of $(A - \sum_{k=1}^{i-1} M_k) \odot S_i$
end for

Example:



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for i ∈ {1, ..., r} do
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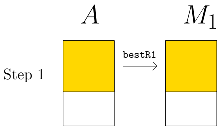

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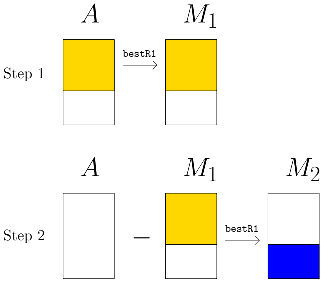

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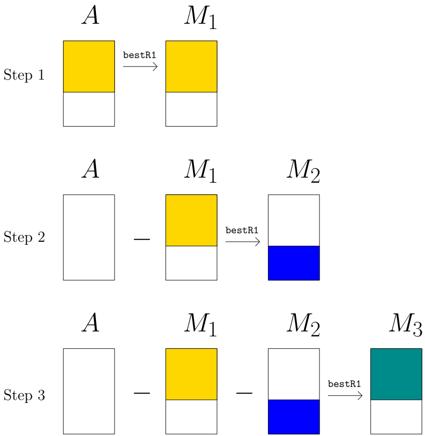


Polynomial solvability characterized by rank-one supports

- The output of the greedy algorithm will always *satisfy the constraints*
- Is the output an optimal solution? Not always

Theorem (2)

If the rank-one supports are pairwise disjoint or identical, then the greedy algorithm gives an optimal solution.

For the same result with a weaker assumption:

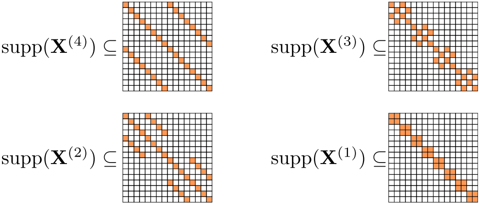
[QT. Le, E. Riccietti, R. Gribonval, **Spurious Valleys, NP-hardness, and Tractability of Sparse Matrix Factorization With Fixed Support**, SIAM Journal of Matrix Analysis and Applications, In press, 2022.]

Multiple-factors cases: the butterfly factorization

A special case: the butterfly factorization

Approximate **any** matrix by a product of $J \geq 2$ butterfly factors

Let $\mathrm{A} := \mathrm{X}^{(4)}\mathrm{X}^{(3)}\mathrm{X}^{(2)}\mathrm{X}^{(1)}$ such that:

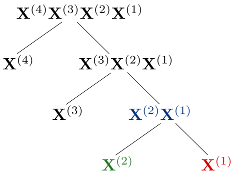


- It is expressive: the composition of matrices with a butterfly structure can accurately approximate any given matrix
- In neural networks faster training and inference time without harming the performance

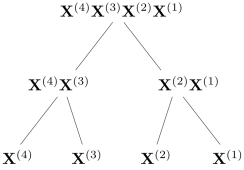
[T. Dao & all. Kaleidoscope: An efficient, learnable representation for all structured linear maps, ICLR, 2020]
[B. Chen & all. Pixelated butterfly: Simple and efficient sparse training for neural network models, PMLR, 2022]

Butterfly factorization: theoretical guarantees

Hierarchical approach:Use our algorithm to recover the partial factors: solve a sequence of two factors problems, if the supports are known



Left-to-right tree



Balanced tree

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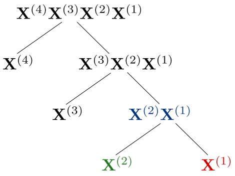

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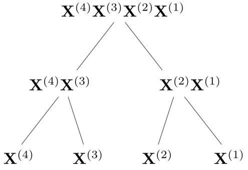


Balanced tree

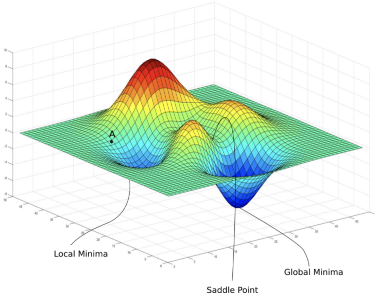
Theorem (3)

If E^* is best error approximation of $A \in \mathbb{R}^{N\times N}$, the solution of the hierarchical algorithm yields a distance/error E such that:

- *Any tree:* $E \leq (N/2 - 1) \times E^*$.
- *Left-to-right (or right-to-left) tree:* $E \leq N^c \times E^*$ *where* $c = \log_4 3 < 1$.

Study of the landscape of the loss function

$$L(X,Y) = \|A - XY^T\|_F^2$$



Has been studied for:

- linear and shallows neural networks
- matrix sensing, phase retrieval, matrix completion ...

[Q. Li, Z. Zhu, G. Tang, **The non-convex geometry of low-rank matrix optimization**, Information and Inference, 2018]
[Z. Zhu & all. **The global optimization geometry of shallow linear neural networks**, JMIV, 2019]
[L. Venturi, A. S. Bandeira, J. Bruna, **Spurious valleys in one-hidden-layer neural network optimization landscapes**, JMLR, 2019]

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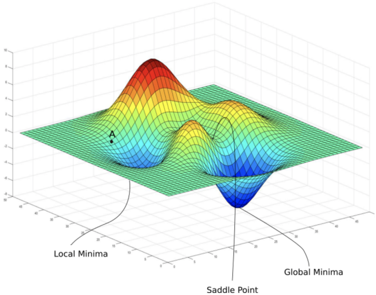

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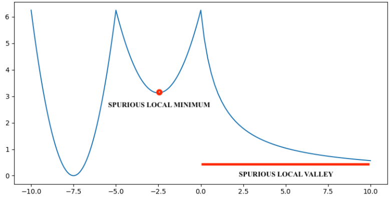
Never with support constraints!

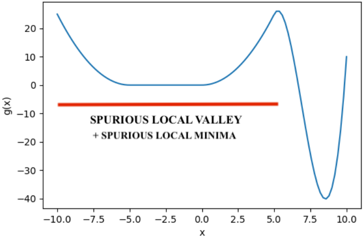
Undesirable spurious objects

Example of undesirable spurious objects :

- Spurious local minima: local minima (but not global minima)
- Spurious local valleys: less known but equally troublesome

[L. Venturi, A. S. Bandeira, J. Bruna, **Spurious valleys in one-hidden-layer neural network optimization landscapes**, JMLR, 2019]





Example of spurious local minimum and spurious local valley. Two undesirable objects: may make the convergence of iterative methods difficult

Landscape of full support matrix factorization

- With unconstrained (full support) matrix factorization:

$$\underset{X\in\mathbb{R}^{m\times r}, Y\in\mathbb{R}^{n\times r}}{\text{Minimize}} L(X,Y) = \|A - XY^\top\|^2$$

- The landscape of $L(X,Y)$ is *benign*:
  - No spurious local minima.[1]
  - No spurious local valleys [2]

[1] [Z. Zhu & all. **The global optimization geometry of shallow linear neural networks**, JMIV, 2019]

[2] [L. Venturi, A. S. Bandeira, J. Bruna, **Spurious valleys in one-hidden-layer neural network optimization landscapes**, JMLR, 2019]

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→ Are there other instances similar to full support matrix factorization ?

[1] [Z. Zhu & all. **The global optimization geometry of shallow linear neural networks**, JMIV, 2019]

[2] [L. Venturi, A. S. Bandeira, J. Bruna, **Spurious valleys in one-hidden-layer neural network optimization landscapes**, JMLR, 2019]

Landscape of $L(X, Y)$ under sparsity constraints

Reminder : Fixed support matrix factorization

$$\underset{X \in \mathbb{R}^{m \times r}, Y \in \mathbb{R}^{n \times r}}{\text{Minimize}} \quad L(X, Y) = \|A - XY^\top\|^2$$

$$\text{Subject to:} \quad \mathrm{supp}(X) \subseteq S_X$$
$$\mathrm{supp}(Y) \subseteq S_Y$$

Theorem (4)

If (S_X, S_Y) satisfy the condition of polynomial solvability in Theorem (2), then for all A, the landscape of $L(X, Y)$ does not contain any spurious local minimum and spurious local valley.

Conclusions

Take home message

For Fixed support matrix factorization (FSMF), we have:

1) It is NP-hard to solve
2) Easy instances with effective direct algorithm exists, competitive with gradient descent.
3) Those easy instances have benign landscape
4) Multiple factors can be dealt with by a hierarchical approach.

On-going works/perspectives

- Study the closedness of the set of solutions to FSMF.
- Can we enlarge the family of tractable instances of FSMF?
- Can we improve the approximate factor in the case of *butterfly factorization*?

Available: an implementation of the algorithm in C++ via Python and Matlab wrappers FAμST toolbox at `https://faust.inria.fr/`.

To know more:

- Q.-T. Le, E. Riccietti, and R. Gribonval (2022), Spurious Valleys, Spurious Minima and NP-hardness of Sparse Matrix Factorization With Fixed Support, *arXiv preprint*, arXiv:2112.00386.
- L. Zheng, E. Riccietti, and R. Gribonval (2022), Efficient Identification of Butterfly Sparse Matrix Factorizations, *arXiv preprint*, arXiv:2110.01235.
- Q.-T. Le, L. Zheng, E. Riccietti, and R. Gribonval (2022), Fast learning of fast transforms, with guarantees, *ICASSP 2022*

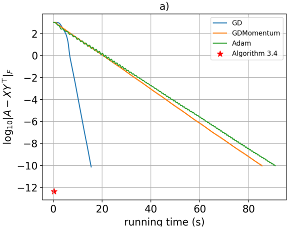
Definition: spurious local valleys

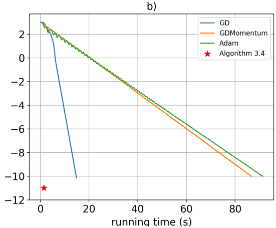
Definition (Spurious local valley - Informal)

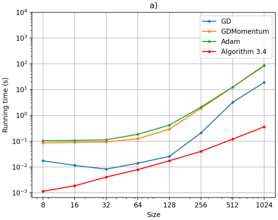
$S \in \mathbb{R}^d$ is a spurious local valley if for all $x \in S$, there does not exist any *continuous path* connecting x and a global minimum x^* *without increasing* the loss function f.

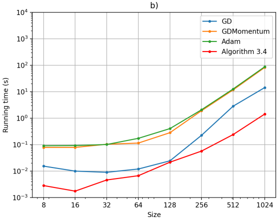
Numerical results: 2 factors

A the Hadamard matrix of size $2^J \times 2^J$, $J = 10$, two different supports





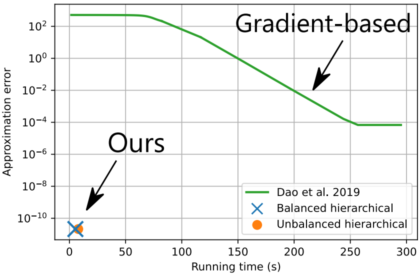




Numerical results: J factors

Approximation of the DFT matrix by a product of $J = 9$ butterfly factors.

Faster and more accurate in the noiseless setting



Also more robust in the noisy setting