Expressivity, sparsity and identifiability in deep neural networks

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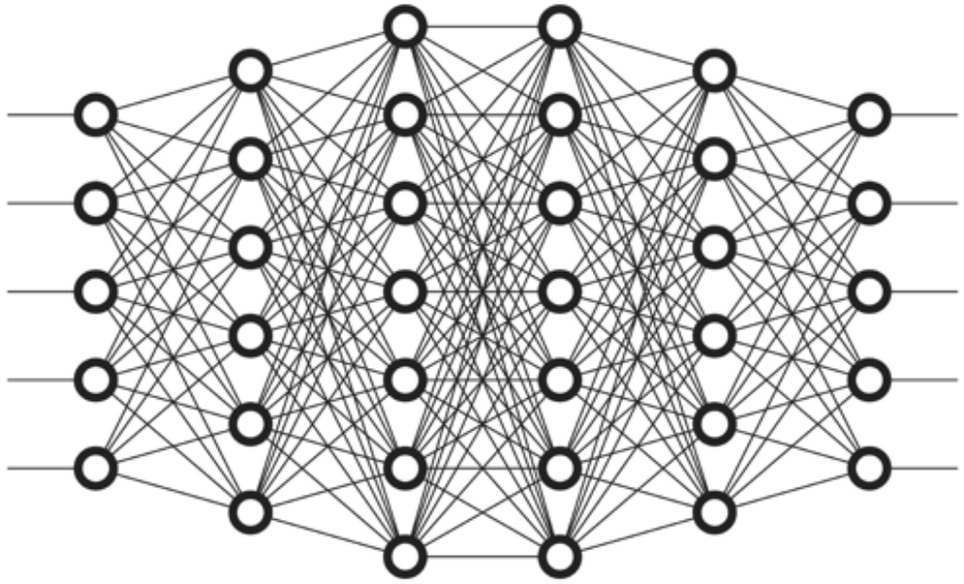
and also: Hakim Hadj-Djilani, Nicolas Bellot, Thomas Gautrais, Adrien Leman, …

Introduction

- Deep neural networks = rich computational architecture
  - ***Expressive***: can implement classical “engineered” workflows
  - ***Tunable***: via optimization on (large) training datasets
  - ***Empirically successful*** … ***yet opaque & resource-hungry***



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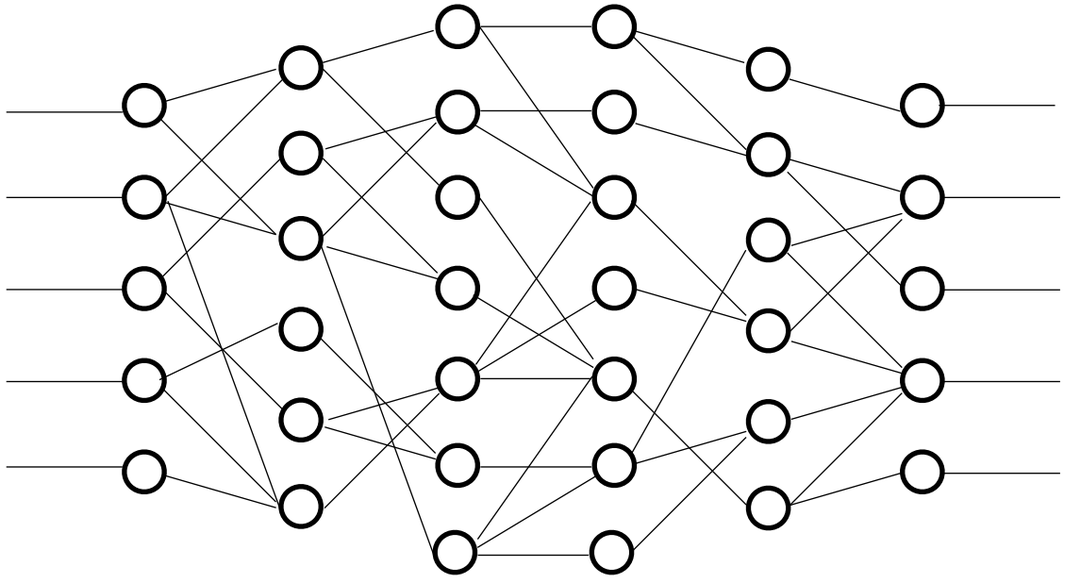
Sparsity as a swiss-knife ?

Interpretability ?
Provably good learning ?
Resource-efficiency ?



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- **Sparsity: some lessons from inverse problems**
- Two-layer sparsity and beyond
- Rescaling-invariance in ReLU networks
- An embedding of ReLU networks

Sparsity in data processing

- As a natural **objective**: frugality / compression
- As a **prior**: identification of latent variables

  - *Prime example* = ***linear inverse problems***

    - linear model $y = \mathbf{A}x$ with known $m \times n$ matrix where $m \ll n$
    - under-determined / ill-posed / infinitely many solutions

  - under sparsity prior $\|x\|_0 \leq k$ and assumptions on $\mathbf{A}$

    - identifiability
    - guaranteed identification with tractable algorithms (e.g. L1 minimization)
    - stable and robust recovery

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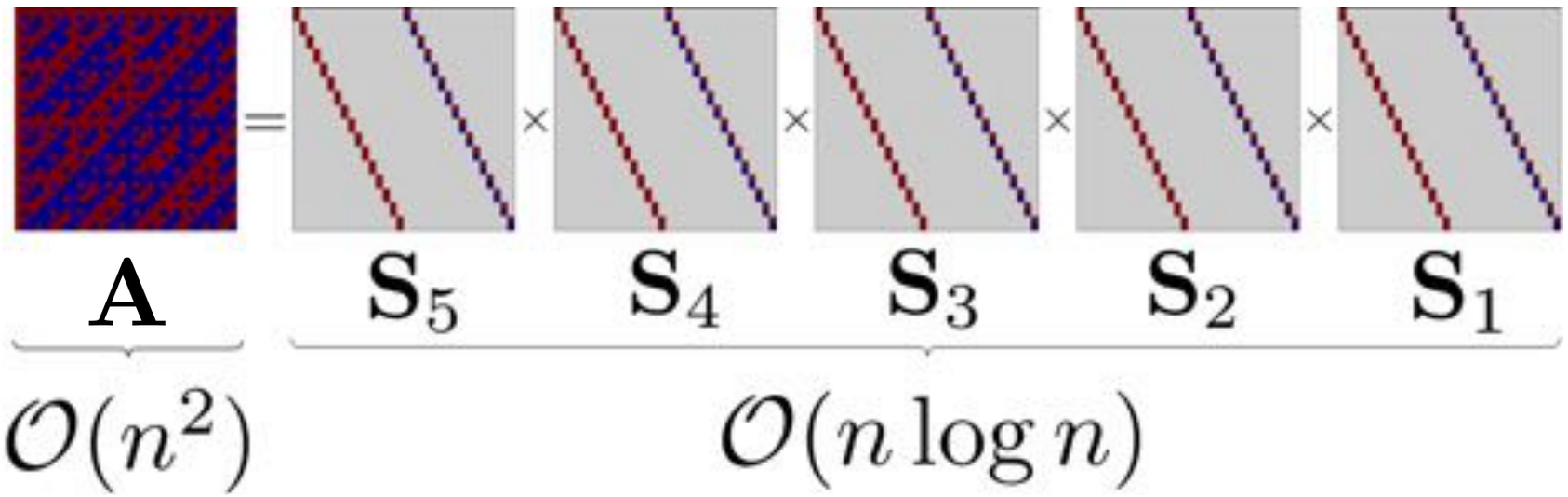
- ***Sparsity beyond linear inverse problems ?***

Fast transforms as sparse factorizations

- **Analytic transforms** (Fourier, wavelets, Hadamard, DCT …) are **fast** because …

Fast transforms as sparse factorizations

- **Analytic transforms** (Fourier, wavelets, Hadamard, DCT …) are **fast** because … **of factorizable structure**[1]



[1] [J. Morgenstern, **The Linear Complexity of Computation**, *J. ACM*, 1975]

Learning Multilayer-Sparse Transforms

- **Products of sparse factors**
  - covers standard fast transforms
  - immediate benefits:
    - **Speed**: *inverse problems and more*
    - **Storage**: *embedded implementation, efficient transmission*

$$\prod_{j=1}^{J} \mathbf{S}_j$$

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- **Principle:** given matrix $\mathbf{A}$, find an approximation

$$\mathbf{A} \approx \prod_{j} \mathbf{S}_j$$

[O. Chabiron & al, **Toward Fast Transform Learning**, *IJCV*, 2014]

[L. Le Magoarou & R. G., **Flexible Multi-layer Sparse Approximations of Matrices and Applications**, *IEEE JSTSP*, 2016]

[T. Dao & al, **Learning Fast Algorithms for Linear Transforms Using Butterfly Factorizations**, *ICML,* 2019]

[Q.T.-Le & R.G., **Structured Support Exploration For Multilayer Sparse Matrix Factorization,**, *ICASSP,* 2021]

Factorization via optimization ?

- **Optimizing a factor given all others**

$$\min \|\mathbf{S}_j\|_1 \text{ s.t. } \mathbf{A} = \mathbf{L}\mathbf{S}_j\mathbf{R}$$

$$\mathbf{L} = \mathbf{S}_1 \dots \mathbf{S}_{j-1}$$
$$\mathbf{R} = \mathbf{S}_{j+1} \dots \mathbf{S}_J$$

- **Sparsity via a global optimization principle ?**

$$\min \sum_j \|\mathbf{S}_j\|_1 \text{ s.t. } \mathbf{A} \approx \Pi_j \mathbf{S}_j$$

  - guarantees ?

Example: blind sparse deconvolution

- **Goal = recover sparse signals from a convolution**

$$\mathbf{a} = \mathbf{s}_1 \star \mathbf{s}_2$$

  - Expressed as $\mathbf{A} = \mathbf{S}_1 \mathbf{S}_2$ (circulant/Toeplitz structure)
  - Easy if one signal is known, e.g. with

$$\min \|\mathbf{s}_2\|_1 \text{ s.t. } \mathbf{a} = \mathbf{s}_1 \star \mathbf{s}_2$$

  - « Natural » blind approach

$$\min \|\mathbf{s}_1\|_1 + \|\mathbf{s}_2\|_1 \text{ s.t. } \mathbf{a} = \mathbf{s}_1 \star \mathbf{s}_2$$

A pitfall

- **Theorem** (Benichoux, Vincent & G. 2013)
  - The trivial pair $\mathbf{s}_1 = \mathbf{a},\ \mathbf{s}_2 = \delta_0$ is always a global optimum of

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- **Under the hood**: intrinsic *scaling ambiguity* :
  - Equivalence classes of rescaling-equivalent parameters
    - if $\mathbf{S}_1, \mathbf{S}_2$ is feasible then so is $\lambda \mathbf{s}_1, \mathbf{s}_2/\lambda$ for any scalar
  - Implicit regularization $\min_\lambda \|\lambda \mathbf{s}_1\|_1 + \|\mathbf{s}_2/\lambda\|_1 \propto \sqrt{\|\mathbf{s}_1\|_1 \|\mathbf{s}_2\|_1}$
  - For any feasible pair $\|\mathbf{a}\|_1 \|\boldsymbol{\delta}_0\|_1 = \|\mathbf{a}\|_1 \leq \|\mathbf{s}_1\|_1 \|\mathbf{s}_2\|_1$

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➡Lesson 1: beware of scaling ambiguities

[A. Benichoux, E. Vincent & R. G., **A fundamental pitfall in blind deconvolution with sparse and shift-invariant priors**, *ICASSP*, 2013]

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Learning sparse networks

Inverse problems wisdom

- It is **NP-hard** to find

$$x^\star \in \arg\min \|x\|_0 \text{ s.t.} y = \mathbf{A}x$$

- … but this is **tractable** under sufficient (sparsity) assumptions

- Can be split into two sub-problems
  - ***hard***: select best support

$$I = \text{supp}(x^\star)$$

  - ***easy***: fit coefficients on support

$$\min_{x_I} \|y - \mathbf{A}_I x_I\|_2^2$$

Learning sparse networks

- Standard practice: dense learning & pruning
- « Lottery ticket hypothesis » heuristics
  - given support, SGD training made easy and stable

[J. Frankle & M. Carbin, **The Lottery Ticket Hypothesis: Finding Sparse, Trainable Neural Networks**, *ICLR*, 2019]

[Zhou & al, **Deconstructing Lottery Tickets: Zeros, Signs, and the Supermask**, *NeurIPS*, 2019]

Can this be grounded on some theory ?

➡ begin with ***shallow & linear*** (but **sparse**) networks

Sparse matrix factorization

Constrained optimization problem

$$\min L(\mathbf{X}, \mathbf{Y}) := \|\mathbf{A} - \mathbf{X}\mathbf{Y}\|_F^2$$

$$\mathtt{supp}(\mathbf{X}) \subseteq I, \ \mathtt{supp}(\mathbf{Y}) \subseteq J \qquad (I, J) \in \Sigma^{\mathtt{left}} \times \Sigma^{\mathtt{right}}$$

- Constraint = families of sparsity patterns $\Sigma^{\mathtt{left}}, \Sigma^{\mathtt{right}}$
- Examples
  - set Σ_k of k-sparse matrices
  - set $\Sigma_{k,\mathtt{col}}$ of matrices with k-sparse columns
  - etc.

Known to be NP-hard

- e.g., covers sparse PCA

What if support is fixed ?

- ***Easy*** for classical sparsity (e.g., X known, Y sparse unknown): ***least squares***

To be or not to be tractable

Theorem 1 (hardness)

- Sparse matrix factorization ***with fixed support*** (I, J) is NP-hard

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➡ very different from least squares !

Detailed proofs and condition: see [Q.-T. Le, E. Riccietti & R. G., **Spurious Valleys, Spurious Minima and NP-hardness of Sparse Matrix Factorization With Fixed Support**, submitted]

[N. Gillis & F. Glineur, **Low-rank matrix approximation with weights or missing data is NP-hard**. *SIAM JMAA,* 2010]
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Theorem 2 (easy instances)

- Under some condition on (I, J),
  - There is an ***efficient algorithm*** to compute a solution
  - For any $\mathbf{A}$, there is ***no spurious local valley***, and essentially ***no spurious local minimum***

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Hardness *vs* landscape ?

Theorem 3

- There exists (I, J) and an explicit open set of matrices such that
  - For each $\mathbf{A}$ in the open set, ***the solution is known analytically***.
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➡ Lesson 2: *there may be life beyond gradient descent!*

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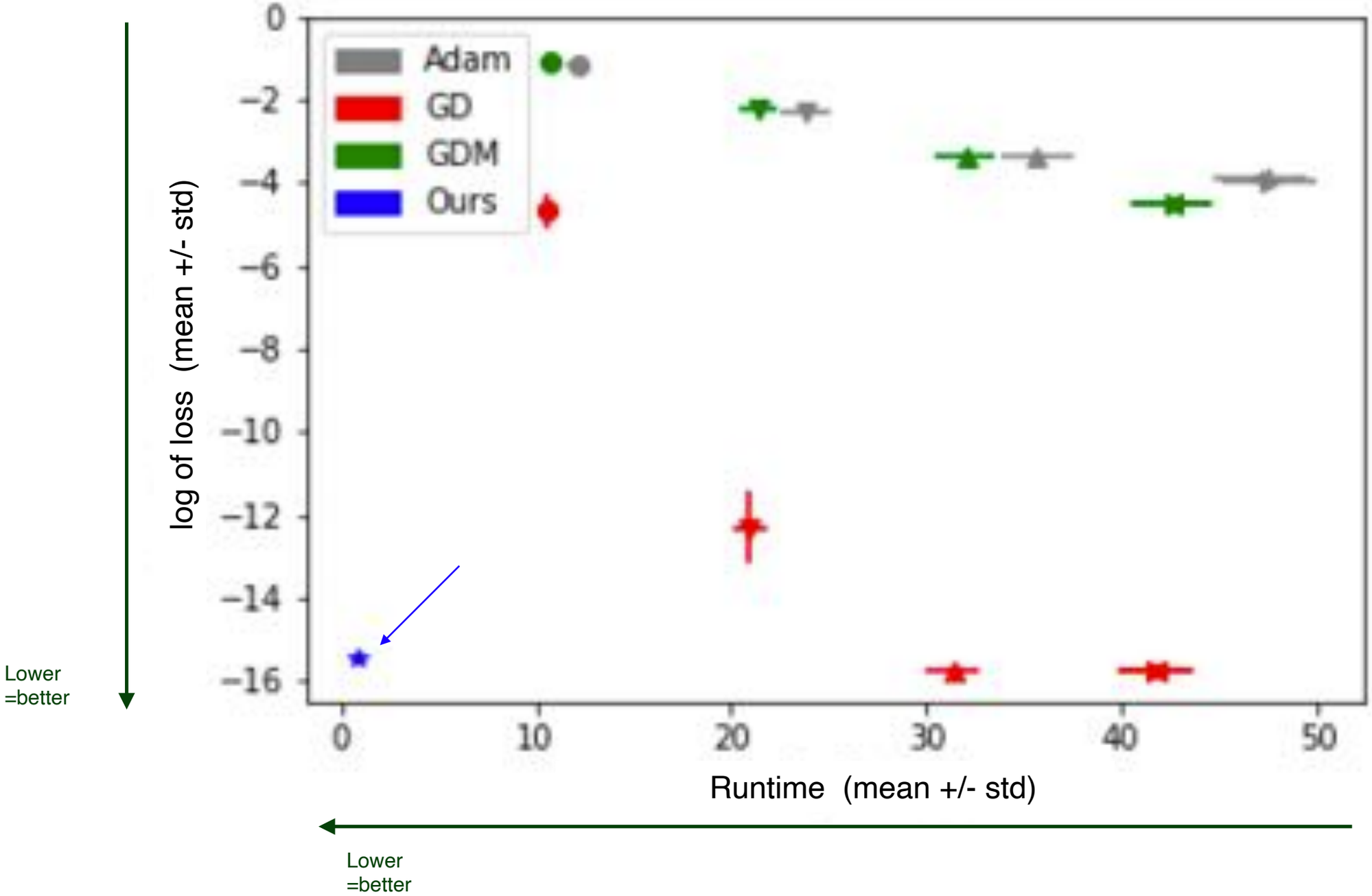
***Indeed*, the algorithm of Theorem 2**

- is ***NOT*** based on gradient-descent
- exploits problem invariances and the SVD

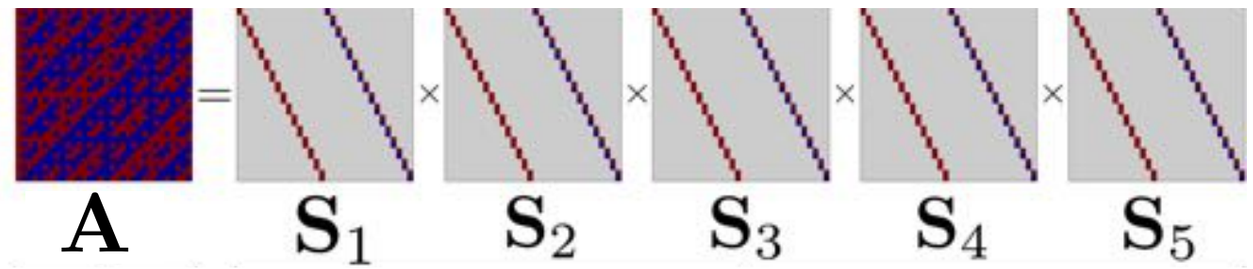
Precision *vs* runtime



GD(M) = gradient descent (with momentum)

Butterfly factorization

- **Butterfly structure**
  - Common sparsity pattern for DCT, DST, DFT, Hadamard



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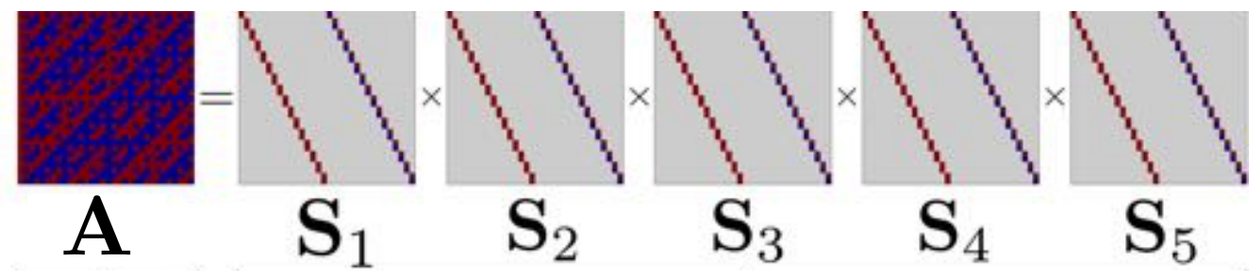
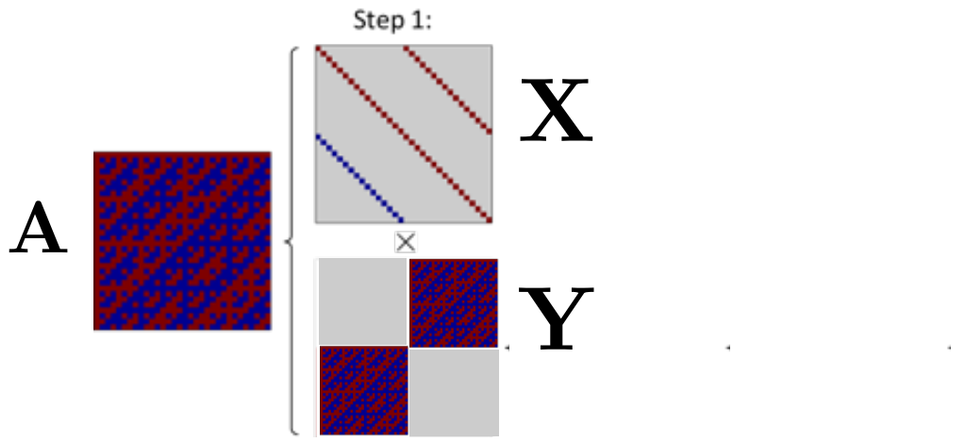


- **Hierarchical factorization approach**



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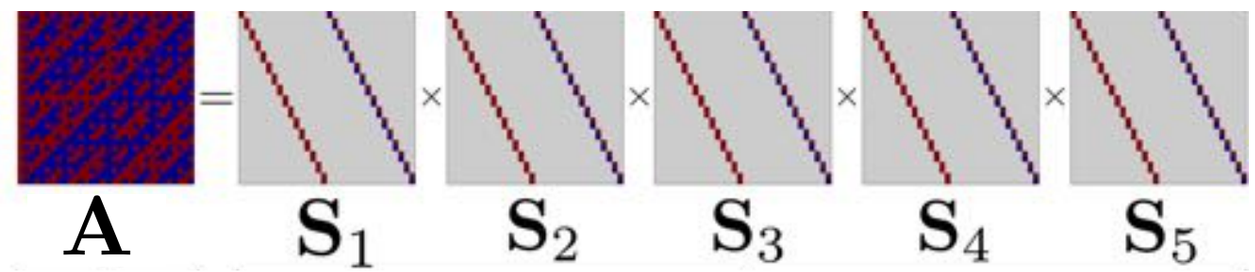

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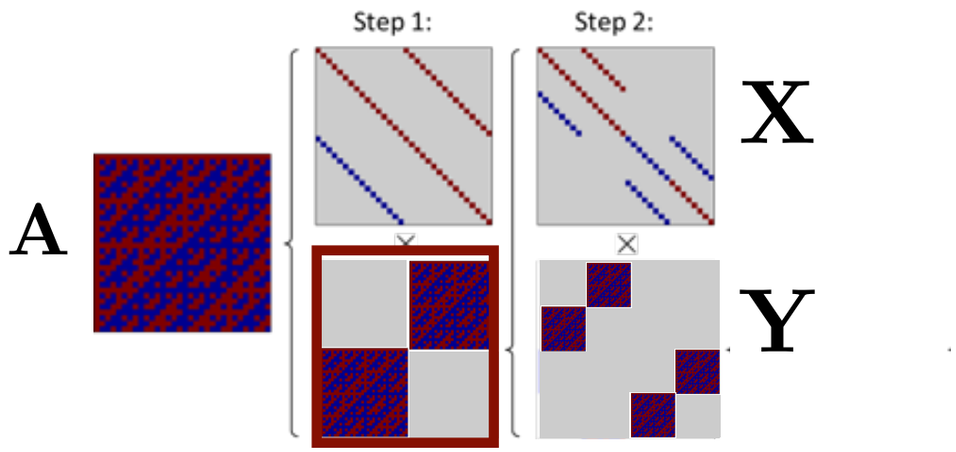

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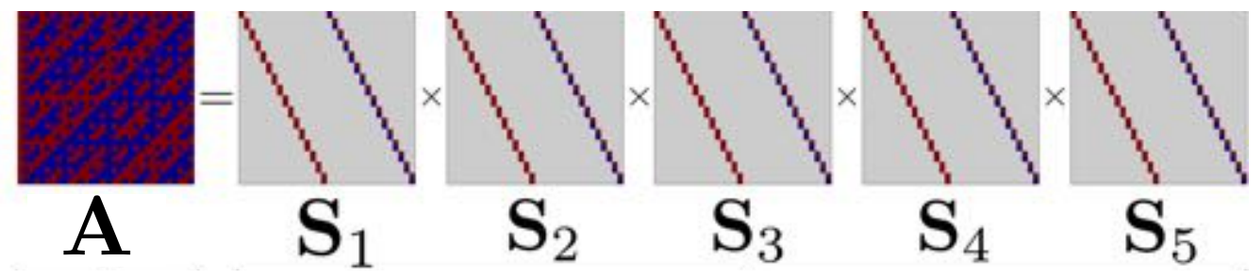

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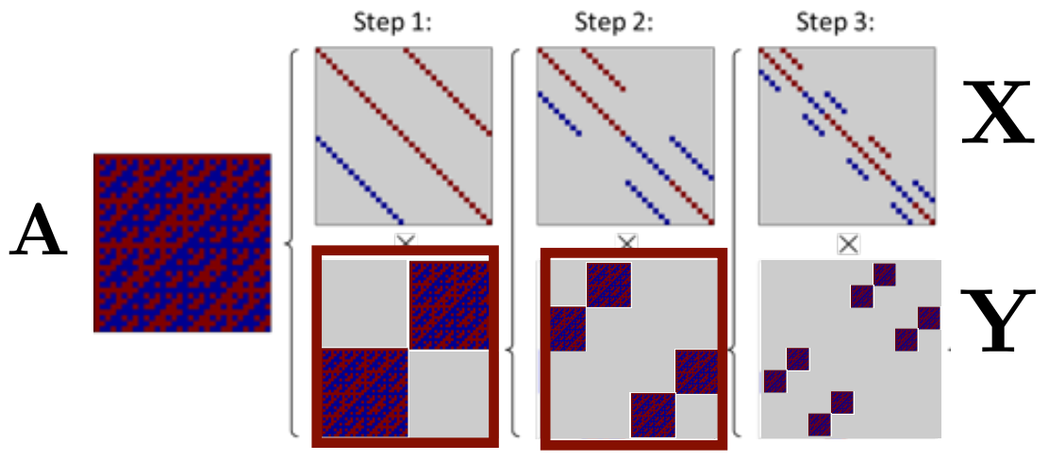

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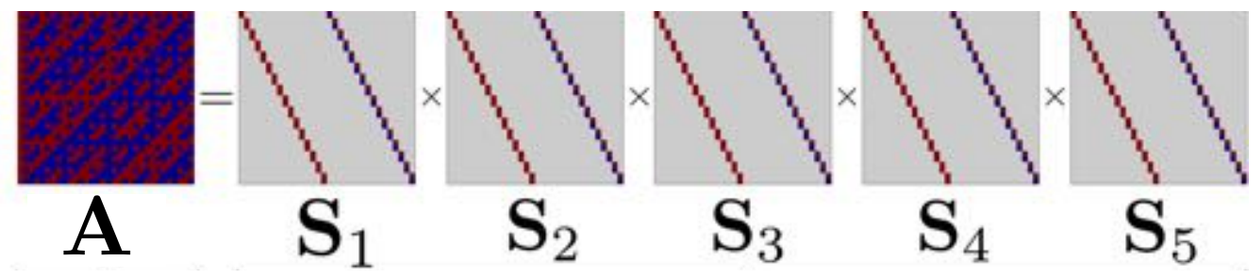

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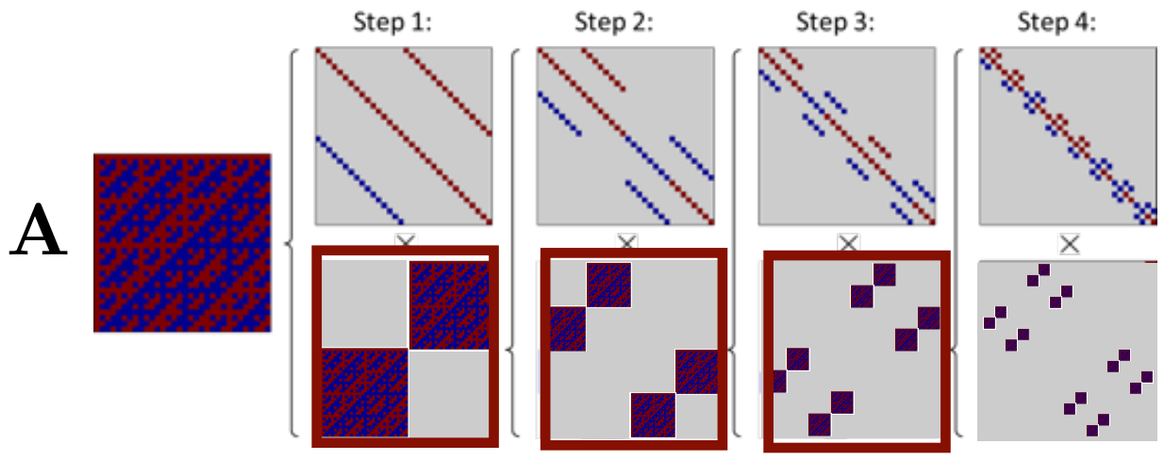

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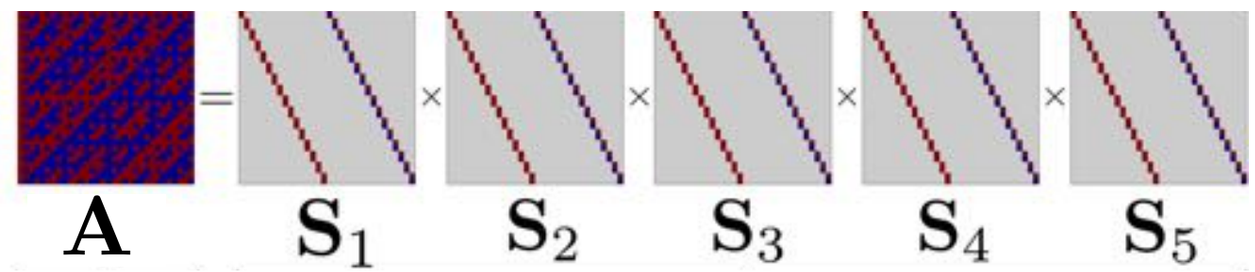

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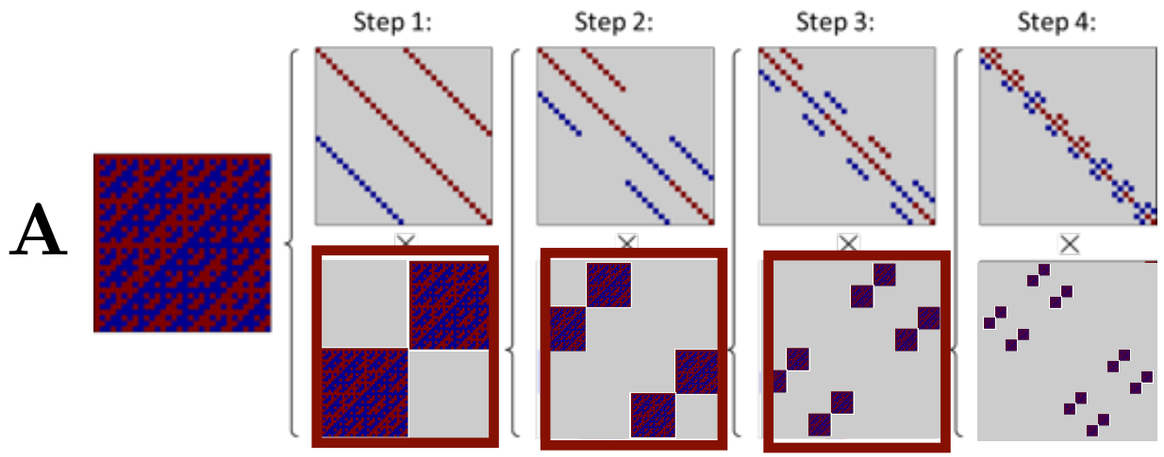

- **Tractability conditions on (I,J) hold at each step**

faust.inria.fr toolbox

-  &  wrappers (C++ core, GPU-compatible)

- PYPI install (or system packages)
  - https://pypi.org/project/pyfaust/
  - `pip install pyfaust`

- Basic usage
  - Convert a matrix to a fast transform
    - e.g. `F = butterfly(A)`
  - Use it transparently (e.g. in inverse problems)
    - essentially replace `x = omp(y,A,k)` with `x = omp(y,F,k)`

    (for selected existing solvers)

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Feedforward neural networks

- **Feedforward network**
  - vector input $x \in \mathbb{R}^d$
  - parameters
    - L affine (“linear”) layers W_ℓ
    - L-1 (hidden) nonlinear layers
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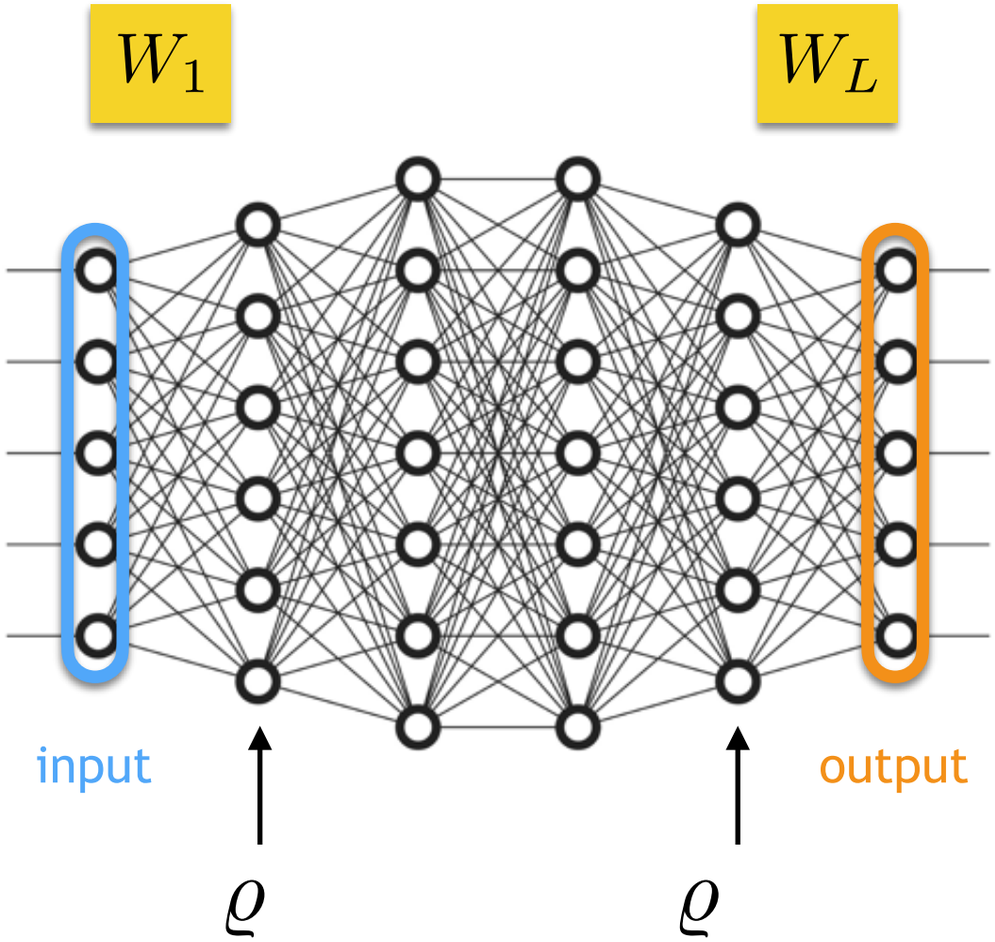

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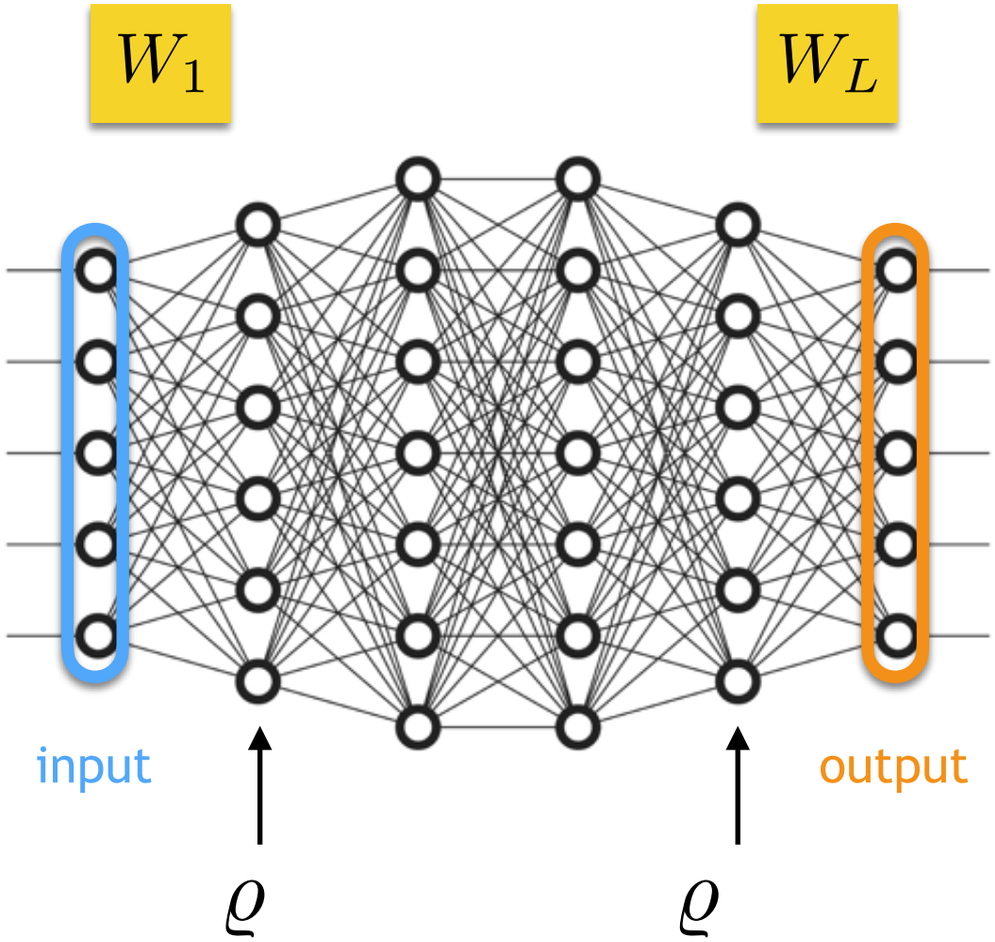
  - ***realization*** $f_\theta : \mathbb{R}^d \to \mathbb{R}^k$



$$f_\theta = W_L \circ \varrho \circ W_{L-1} \circ \cdots \circ \varrho \circ W_1$$

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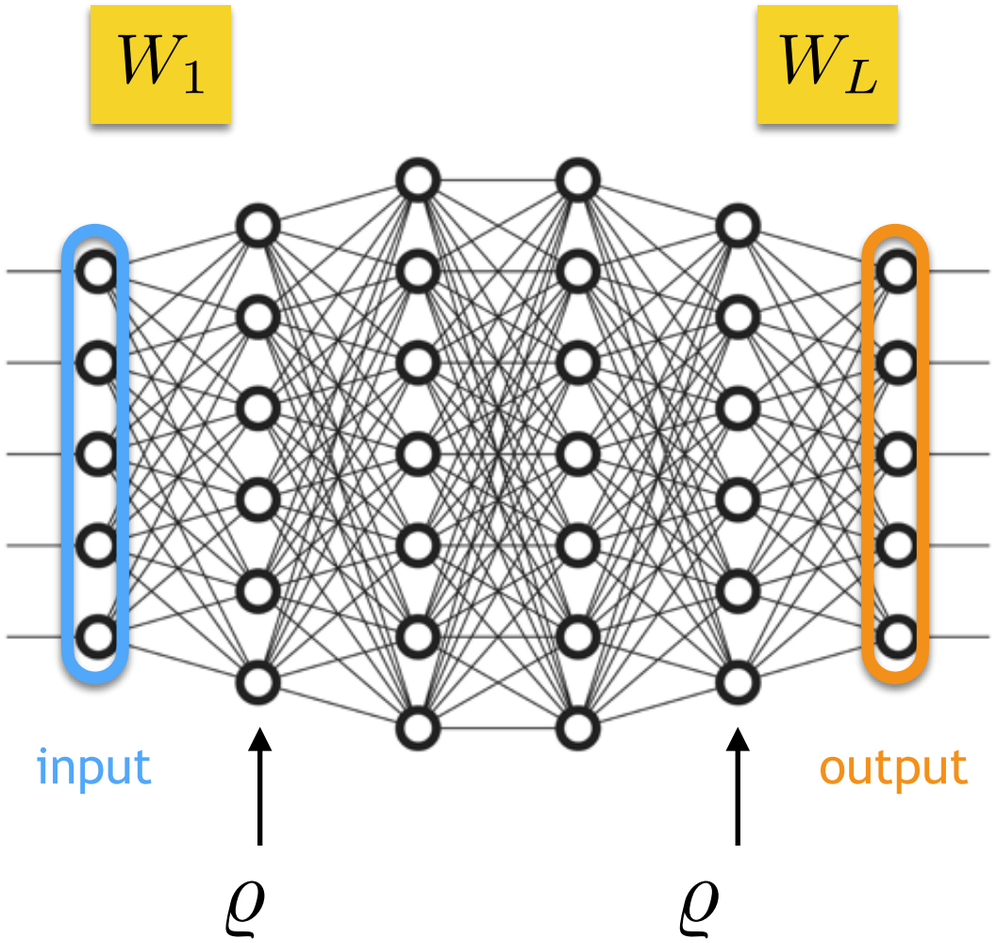


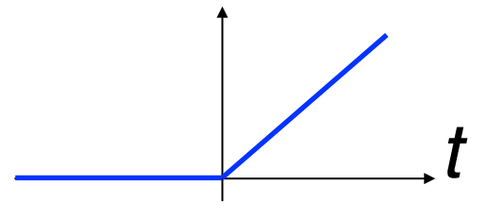
$$f_\theta = W_L \circ \varrho \circ W_{L-1} \circ \cdots \circ \varrho \circ W_1$$

- other ingredients: max-pooling, skip connections, conv … NOT IN THIS TALK

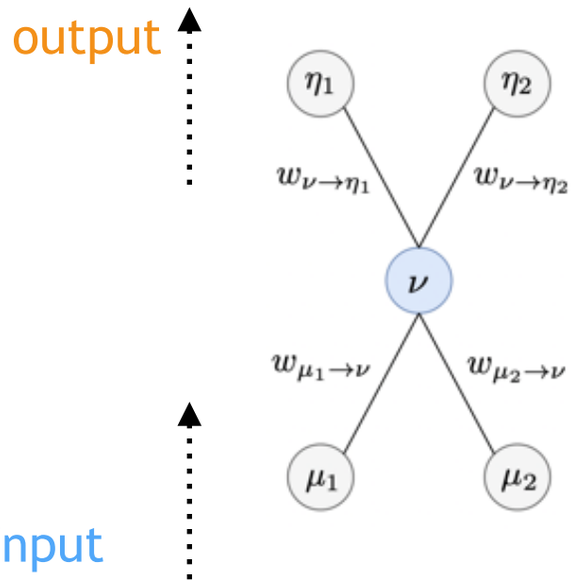
Invariance of ReLU-networks

- **The ReLU is positively homogeneous**

$$\varrho(t) = \texttt{ReLU}(t) = \max(t, 0) = t_+$$



- **Rescaling** incoming/outgoing weights of a neuron



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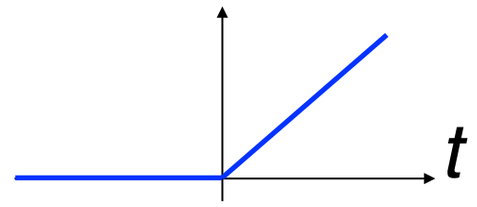
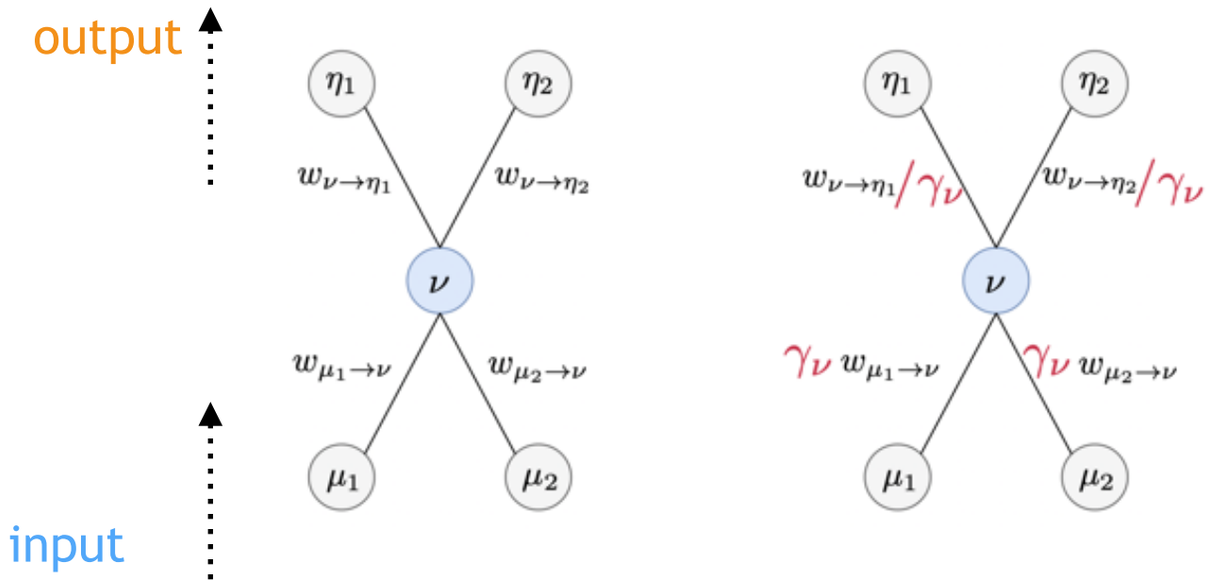


- **Rescaling** incoming/outgoing weights of a neuron



Invariance of ReLU-networks

- **The ReLU is positively homogeneous**

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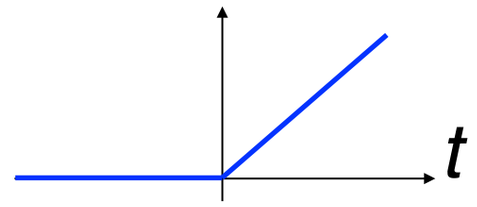

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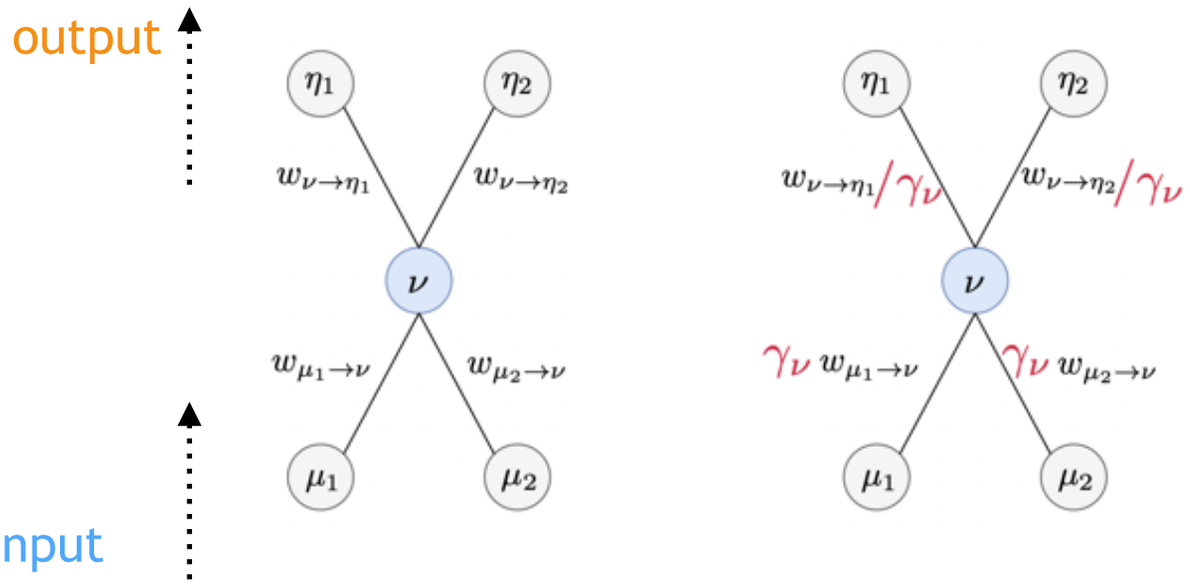

- Notion of **scaling-equivalent parameters** $\theta' \sim_S \theta$
  - implies **functional equivalence** $f_\theta = f_{\theta'}$

Scaling-equivalent parameters …

- … are **always functionally equivalent**
- … but **can behave *wildly* differently**
  - during SGD optimization
    - see e.g. [B. Neyshabur & al, **Path-SGD - Path-Normalized Optimization in Deep Neural Networks**. *NeurIPS,* 2015]
  - under quantization
    - see e.g. [M. Nagel & al, **Data-Free Quantization Through Weight Equalization and Bias Correction**. *ICCV,* 2019]

*Can we **wander** in the equivalence class to improve some performance measure **without changing the network's prediction ?***

Benefits of scale-invariance: E-norm

- **Context**: stochastic gradient descent (SGD)

https://github.com/facebookresearch/enorm

Benefits of scale-invariance: E-norm

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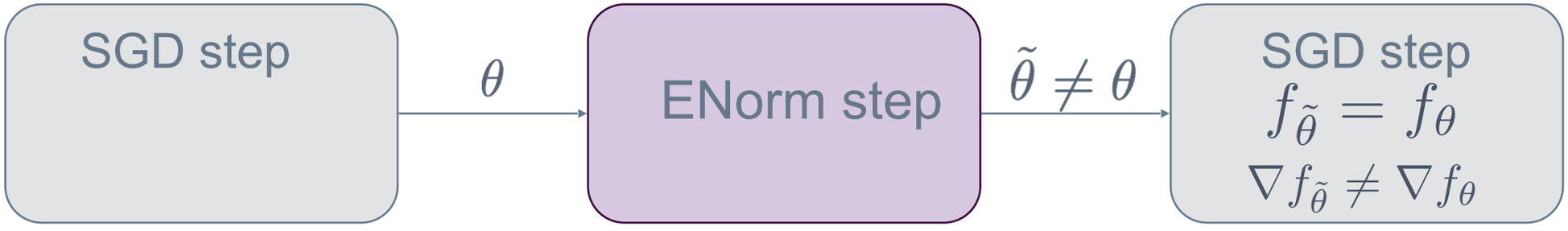

- **Heuristic:** choose a « canonical » representer

$$\tilde{\theta} = \arg \min_{\theta' \sim_S \theta} \|\theta'\|_p$$

  - Lp-norm *on weights* only, any p>0
  - Problem proved to ***equivalent to a convex one***

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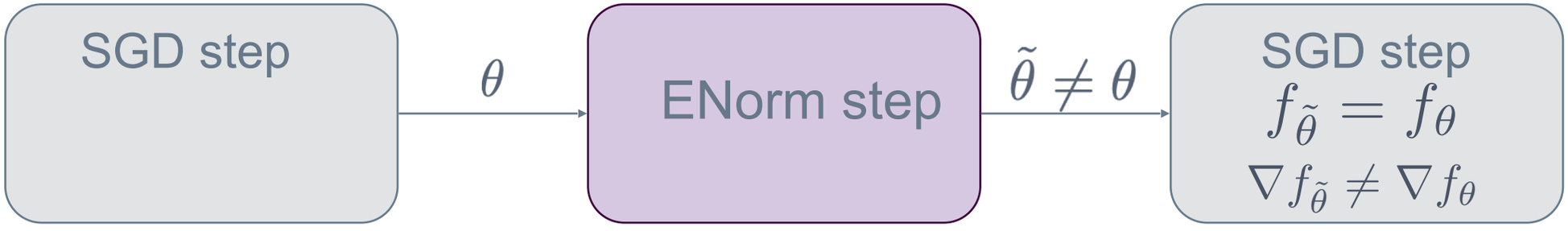

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- **ENorm algorithm**: Fast, Iterative, Sinkhorn*-like
  - block-coordinate descent
  - provably converges to « canonical » representant

*[Sinkhorn & Knopp, 1967]

[P. Stock, B. Graham, R. G. & H. Jégou, **Equi-normalization of Neural Networks**. ICLR, 2019]

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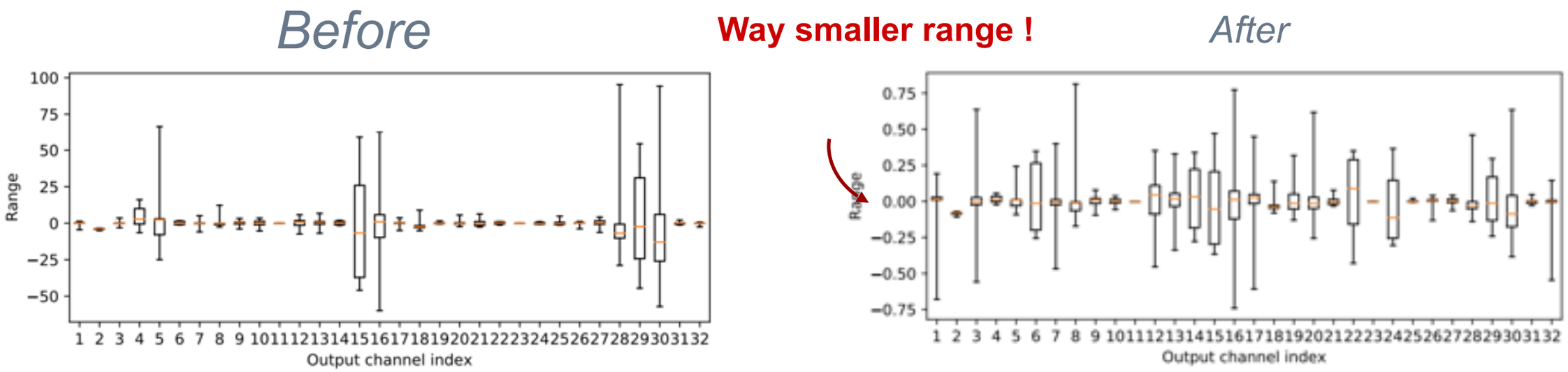
Application to quantization

- [Nagel et al.] leverage ENorm for int8 quantization with Weight Equalization



[Nagel, van Baalen, Blankevoort & Welling, ICCV 2019]
Image credit: Nagel *et al.*

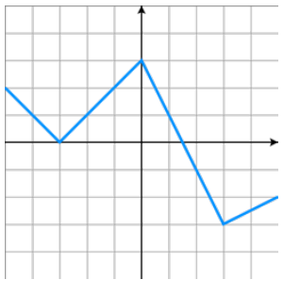
- Lesson 3: ~~beware of~~ scale-invariance !
  (try to) harness

- Sparsity: some lessons from inverse problems
- Two-layer sparsity and beyond
- Scale-invariance in ReLU networks
- **An embedding of ReLU networks**

Realizations of ReLU-networks

- $f_\theta(x)$ **as a function of** x
  - Continuous and piecewise (affine) linear

- **d=1**



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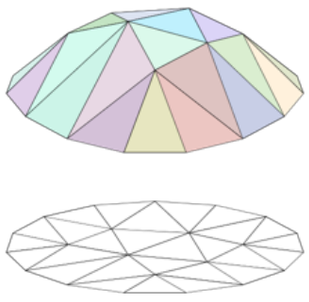

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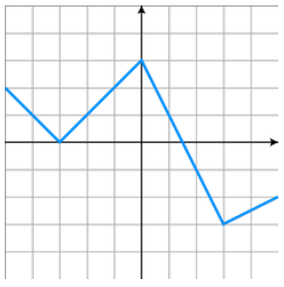

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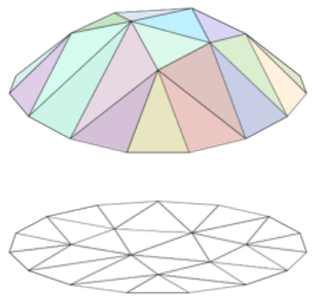

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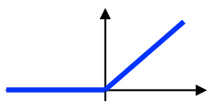

- **Activation vector (hidden neurons)**

$$\mathbf{a}(\theta, x) := \{a_\nu(\theta, x)\}_{\nu \in H} \in \{0,1\}^H$$

  - Linear regions: visible pieces
  - Activation region: *hidden* pieces
    - Do not always coincide

Realizations of ReLU-networks

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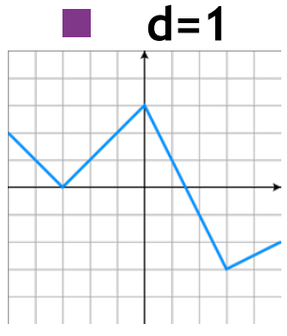

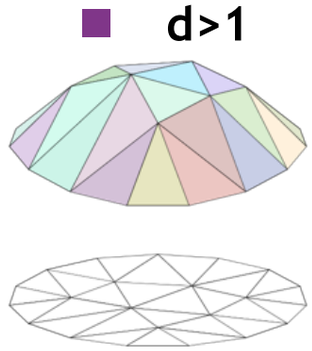

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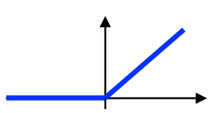

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$f_\theta(x)$ as a function of θ

- Continuous and piecewise polynomial
- In the interior of an *activation region*
  - activation vector is ***locally constant***

$$\theta \mapsto \mathbf{a}(\theta, x)$$

  - realization is *locally polynomial*

$$\theta \mapsto f_\theta(x)$$

Realizations of ReLU-networks

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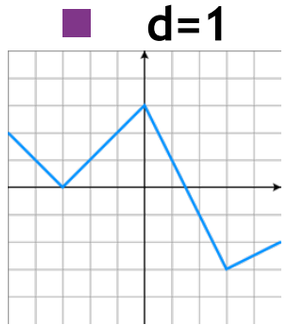

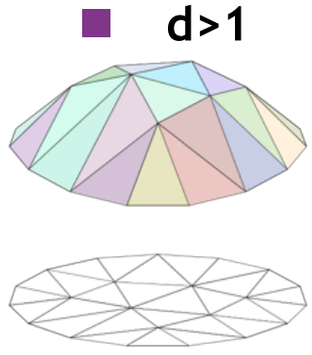

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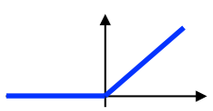

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  - can be written as

$$f_\theta(x) = \langle \bar{\mathbf{a}}(\theta, x), \boldsymbol{\Phi}(\theta) \rangle$$

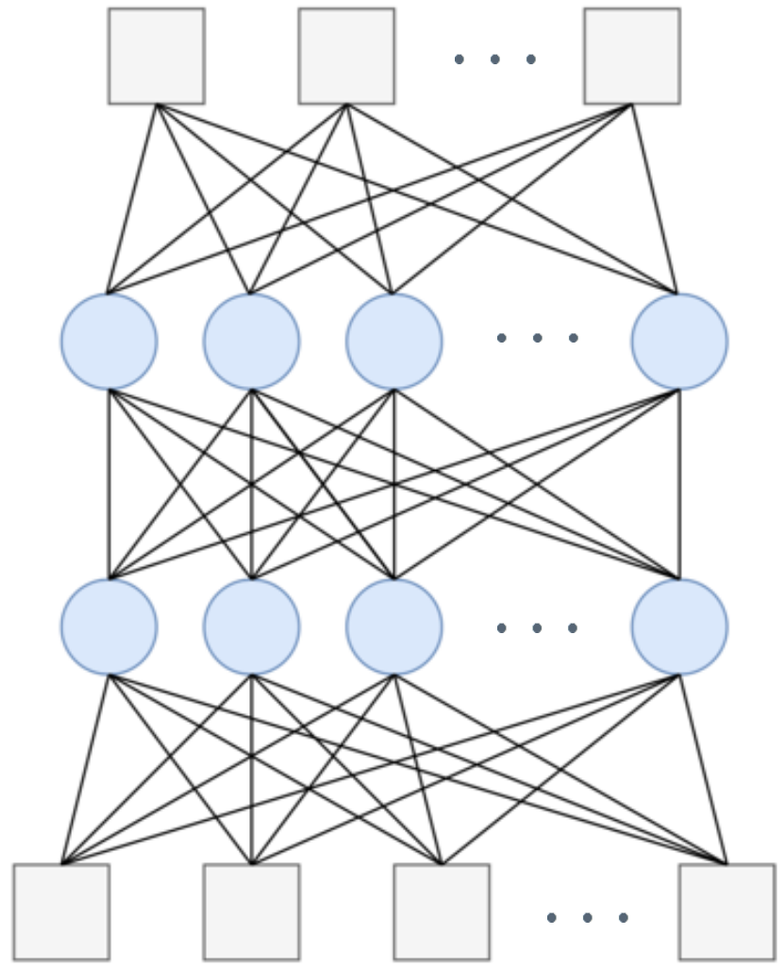
rescaling-invariant embedding

Embedding ReLU network parameters

Architecture

Neurons

Paths



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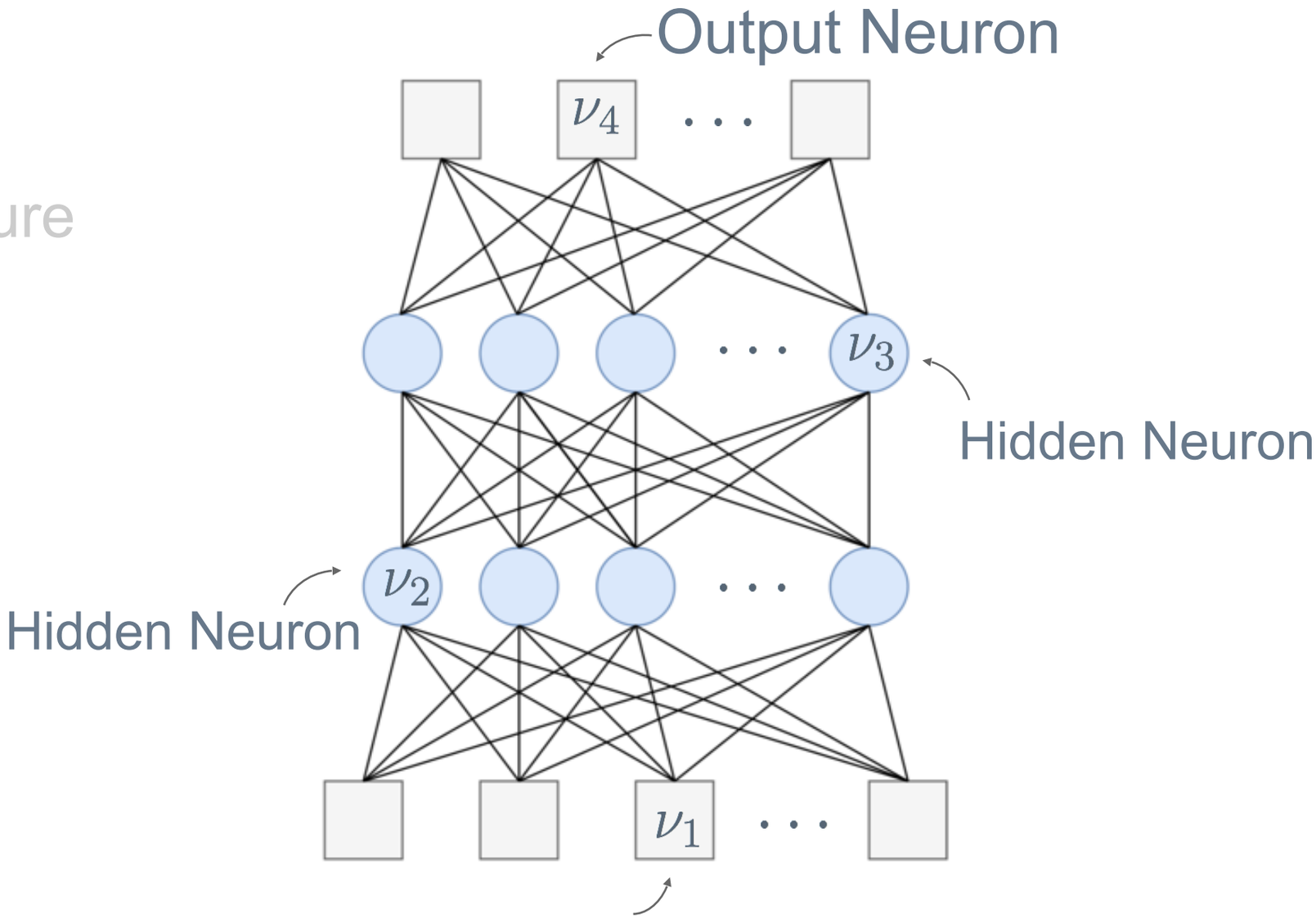

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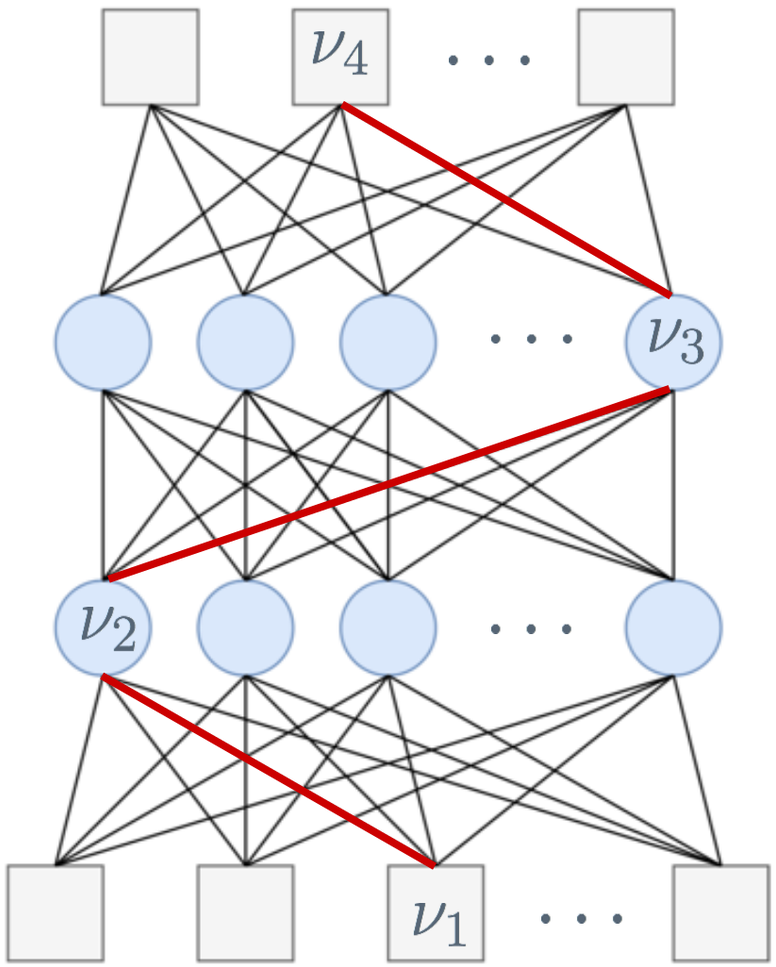

$$p = \nu_1 \to \nu_2 \to \nu_3 \to \nu_4$$

$p \in \mathcal{P}$ *full* path

$$\Phi_p(\theta) := \Pi_{e \in p} w_e$$

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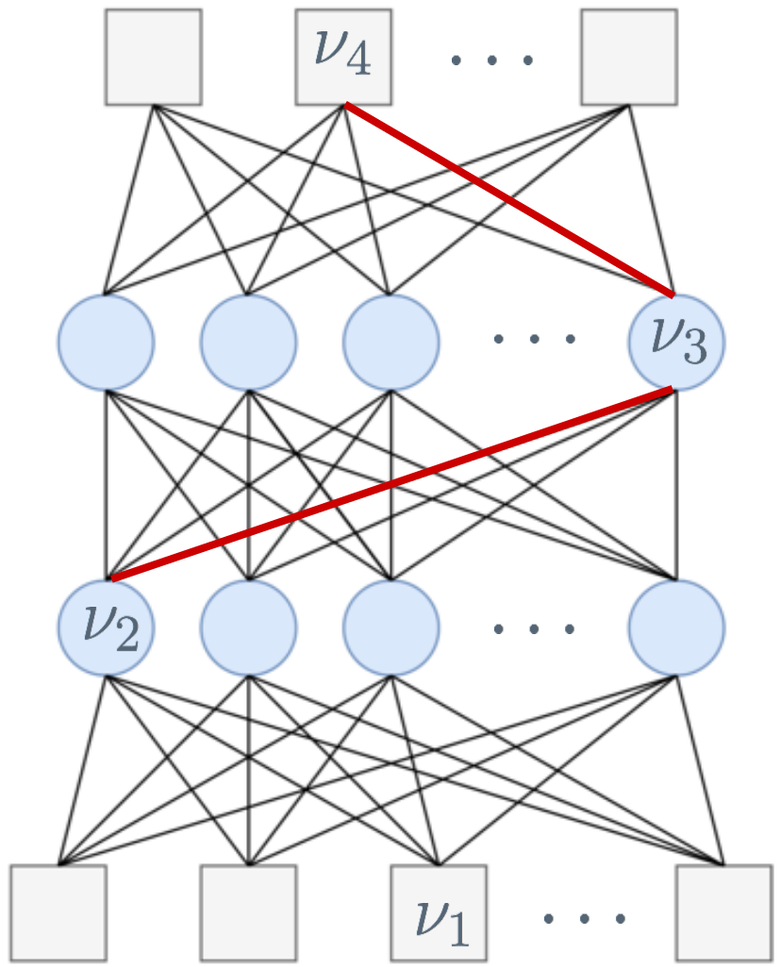

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$$q = \nu_\ell \to \ldots \to \nu_4$$

$q \in \mathcal{Q}$ *partial* path

$$\Phi_q(\theta) := b_\ell \Pi_{e \in q} w_e$$

appears implicitly, without biases,
in [Neyshabur & al 2015]
related idea: Segre embedding with *layerwise* scaling factor, see e.g.
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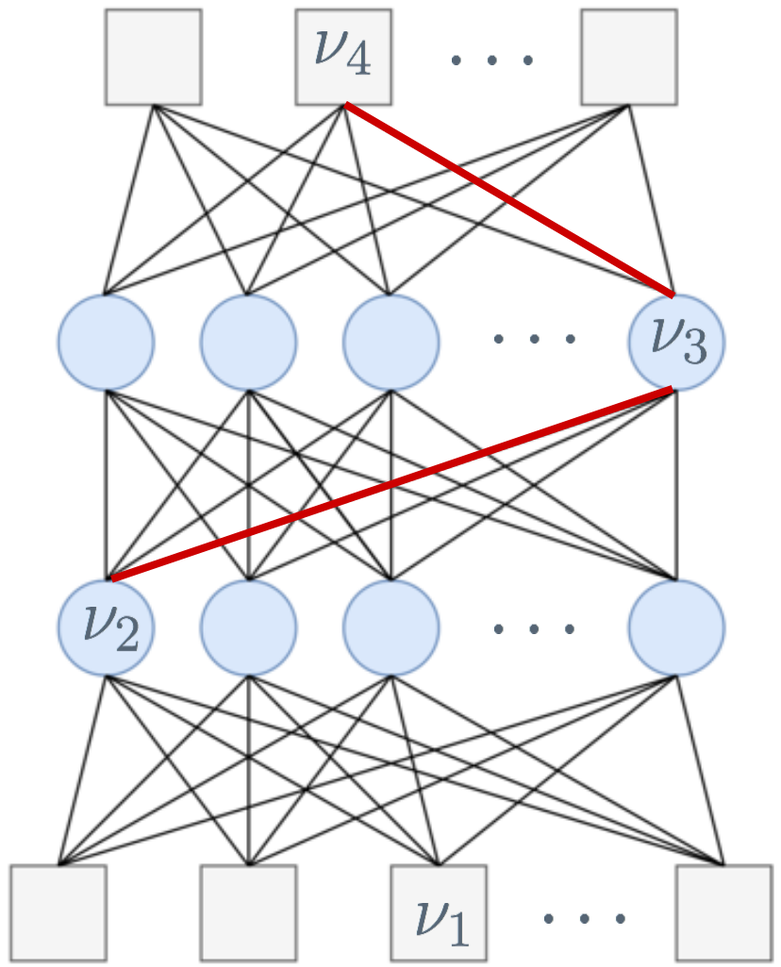

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and similarly: activations of full / partial paths $\bar{a}_p(\theta, x), \bar{a}_q(\theta, x)$

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Reverse-engineering networks ?

- **Scaling-equivalence *vs* functional equivalence ?**
  - One direction always true

$$\theta' \sim_S \theta \xrightarrow{\text{any parameters}} \boldsymbol{\Phi}(\theta') = \boldsymbol{\Phi}(\theta) \xrightarrow{\text{any parameters}} f_{\theta'} = f_\theta \quad \text{on } \mathcal{X} = \mathbb{R}^d$$

$$\texttt{sign}(\theta') = \texttt{sign}(\theta)$$

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  - see e.g. [C. Fefferman, **Reconstructing a neural net from its output**. *Revista Matemática Iberoamericana*, 1994]
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« admissible » parameters

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$\texttt{sign}(\theta') = \texttt{sign}(\theta)$

$f_{\theta'} = f_\theta$ on some finite $\mathcal{X} \subseteq \mathbb{R}^d$

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$f_{\theta'} = f_\theta$ ⇐ globally, up to permutations?

Hard direction = converse

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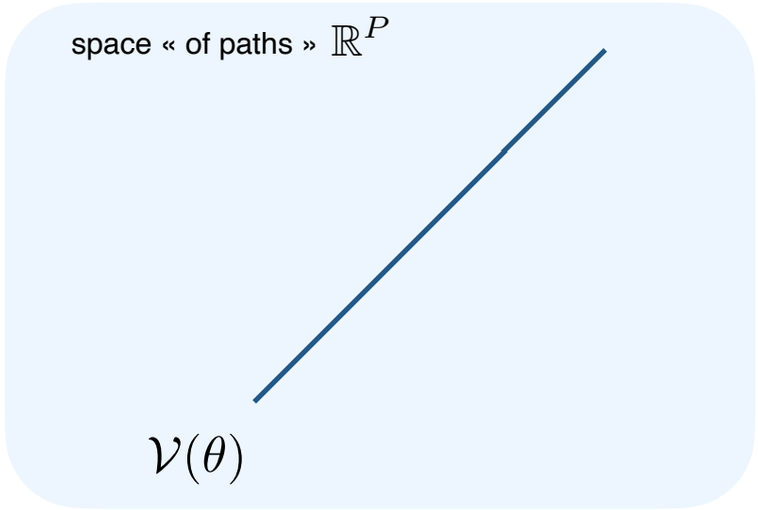
Non-degeneracy

- **Recall** $f_\theta(x) = \langle \bar{\mathbf{a}}(\theta, x), \mathbf{\Phi}(\theta) \rangle$

  binary activation — path-space embedding

- **Definitions**
  - Activation space: $\mathcal{V}(\theta) \approx \mathtt{span}^{\perp}(\bar{\mathbf{a}}(\theta, x), x \in \mathbb{R}^d)$



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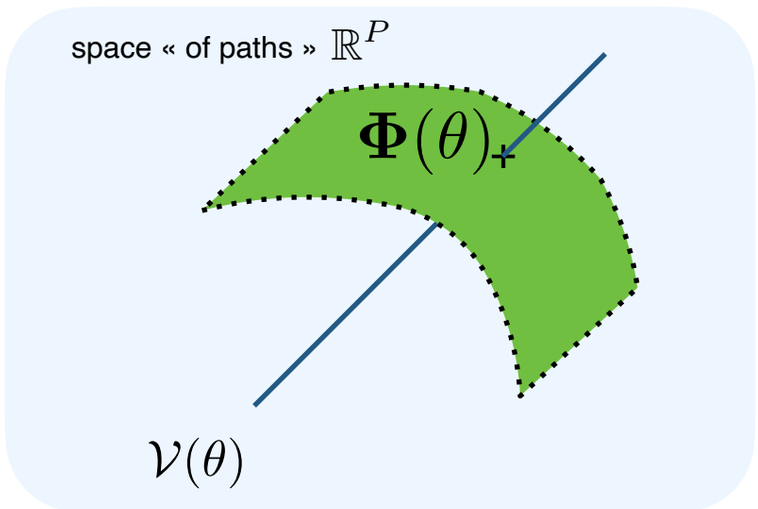
  - **Non-degenerate** parameter: *locally around* θ



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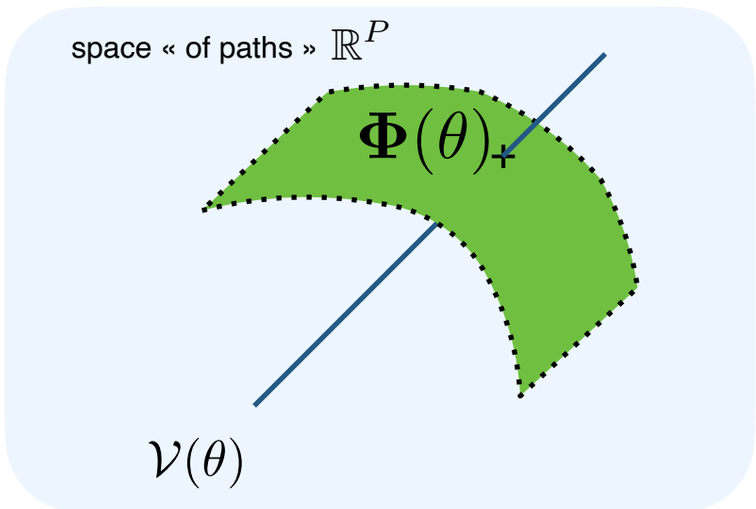
Non-degeneracy



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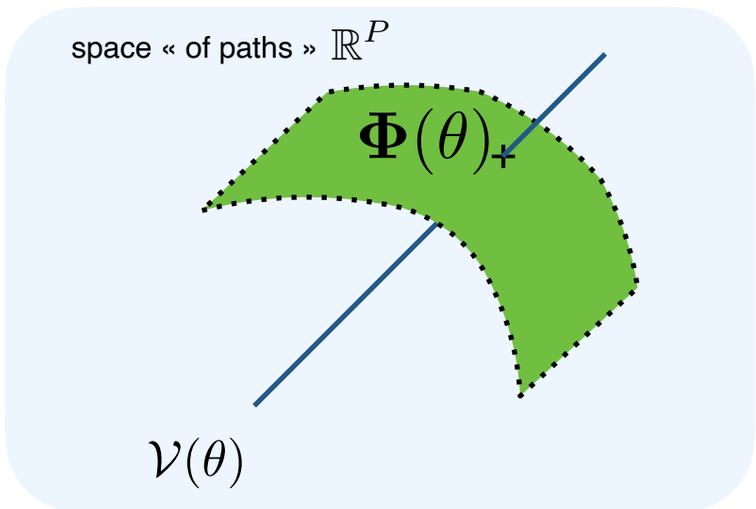
$$f_{\theta'} \overset{\text{on } \mathcal{X}}{=} f_\theta \quad \Longrightarrow \quad \theta' \sim_S \theta$$

  - **size** of the finite set $\mathcal{X}$ linked to dimension of $\mathcal{V}(\theta)$

Non-degeneracy



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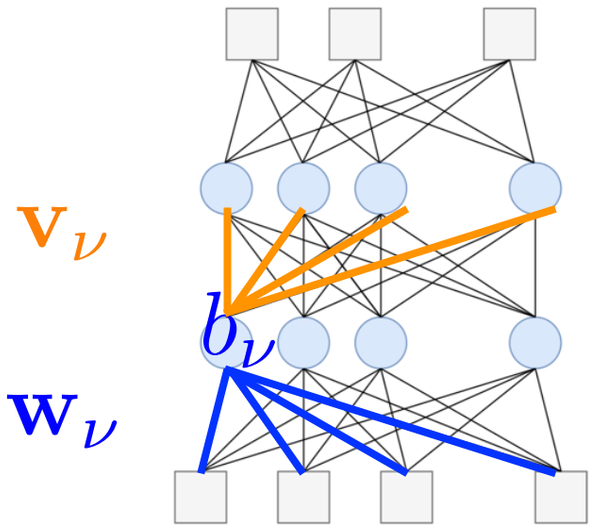
Twin neurons, and irreducibility

- **For each neuron**
  - bias
  - vectors of incoming / outgoing weights



- **Definitions**
  - ***Twin neurons***
    - if $(\mathbf{w}_\nu, b_\nu) = \lambda(\mathbf{w}_{\nu'}, b_{\nu'})$
    - positive / negative twins depending on sign of λ
  - ***Irreducible***
    - if for every subset T of neurons of every layer we have

$$\sum_{\nu \in T} \mathbf{v}_\nu \mathbf{w}_\nu^\top \neq 0$$

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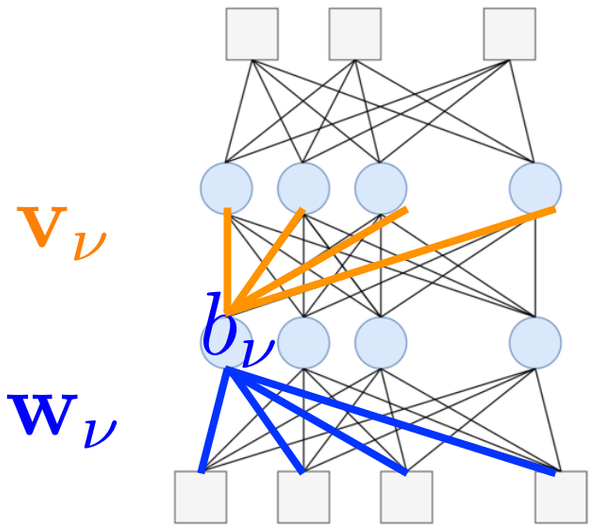

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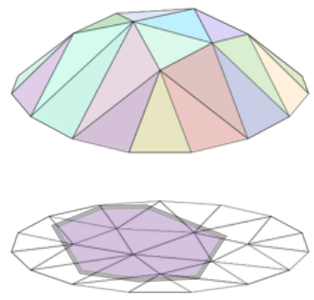
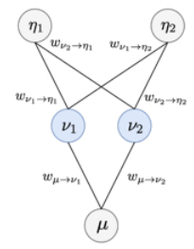
Global identifiability ?

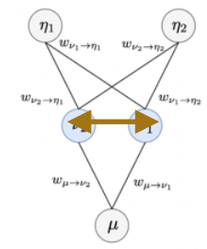
- **Definition: PS-identifiable parameter**
  - up to scaling & ***layerwise permutations***
  - from some set $\mathcal{X} \subseteq \mathbb{R}^d$



θ



θ'



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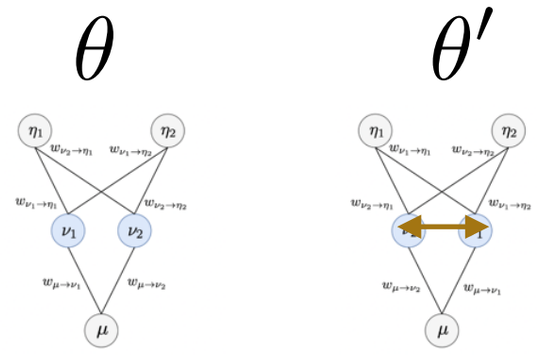
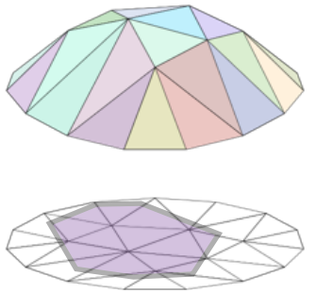
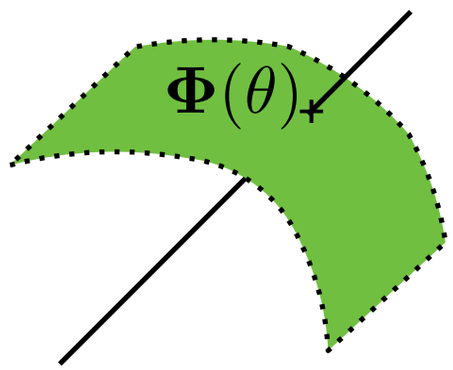




- **Theorem**
  - If θ is PS-identifiable from some $\mathcal{X} \subseteq \mathbb{R}^d$ then
    - It is irreducible
    - It is *locally* identifiable, *up to scaling only*
      - implies absence of *positive* twin neurons
    - Case of *bounded* $\mathcal{X}$: no negative twins either
    - Case of *finite* $\mathcal{X}$: θ is non-degenerate



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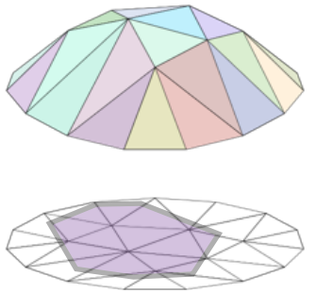

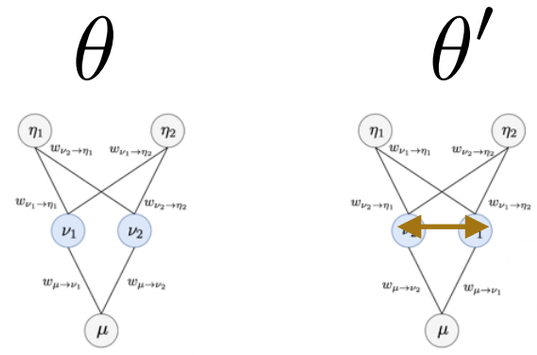

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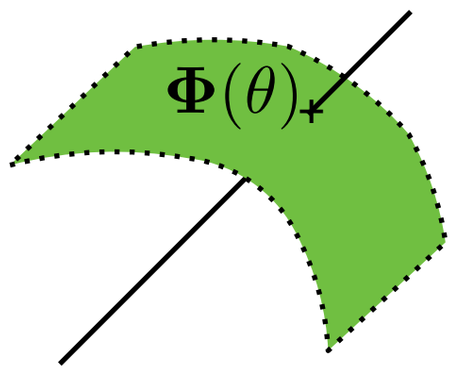

- **Converse for shallow networks:**
  - PS-identifiable from bounded $\mathcal{X}$ **iff** no twins & irreducible

- Sparsity: some lessons from inverse problems
- Two-layer sparsity and beyond
- Scale-invariance in ReLU networks
- An embedding of ReLU networks
- **Wrap-up**

Take Home Messages

- Sparse know-how can break in multilayer setting
  - forget L1 regularization ? beware of rescaling
  - NP-hardness even with fixed, known support
- Life beyond SGD
  - efficient sparse factorization with no gradient descent for certain fixed multilayer sparsity patterns
- Harnessing rescale equivalence in ReLU networks
  - a scale-invariant embedding
  - applications to identifiability analysis

Perspectives

- **Leveraging the full potential of the embedding**
  - Optimization on natural manifold (~path-SGD)
  - Quantization beyond heuristics
  - « Canonical » representer in equivalence class
- **Identifiability: a step towards explainability ?**
  - Characterizing PS-identifiability for deep networks
    - including with convolution layers and/or (structured) sparsity
      - two layer linear sparse: [L. Zheng, E. Riccietti & R. G., **Identifiability in Exact Sparse Matrix Factorization**. *working draft*, 2021]
  - Intuitive meaning of « irreducibility »
  - Sampling complexity and role of activation spaces
- **Beyond ReLU invariances**
  - e.g. in transformers

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Elisa Riccietti

Pierre Stock

Hervé Jégou

Léon Zheng

and also: Hakim Hadj-Djilani, Nicolas Bellot, Thomas Gautrais, Adrien Leman, …