

Dynamic Sparse Training: challenges and opportunities towards scalable, efficient, and sustainable AI

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SMART DIASPORA 2023, TRUST-AI, TIMISOARA

OUTLINE

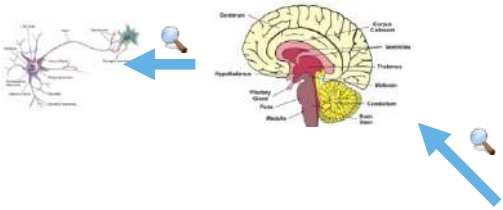
- *Context&Motivation*
- Dense-to-sparse training
- Sparse-to-sparse training
 - principles
 - utilization

SCIENCE PARADIGMS



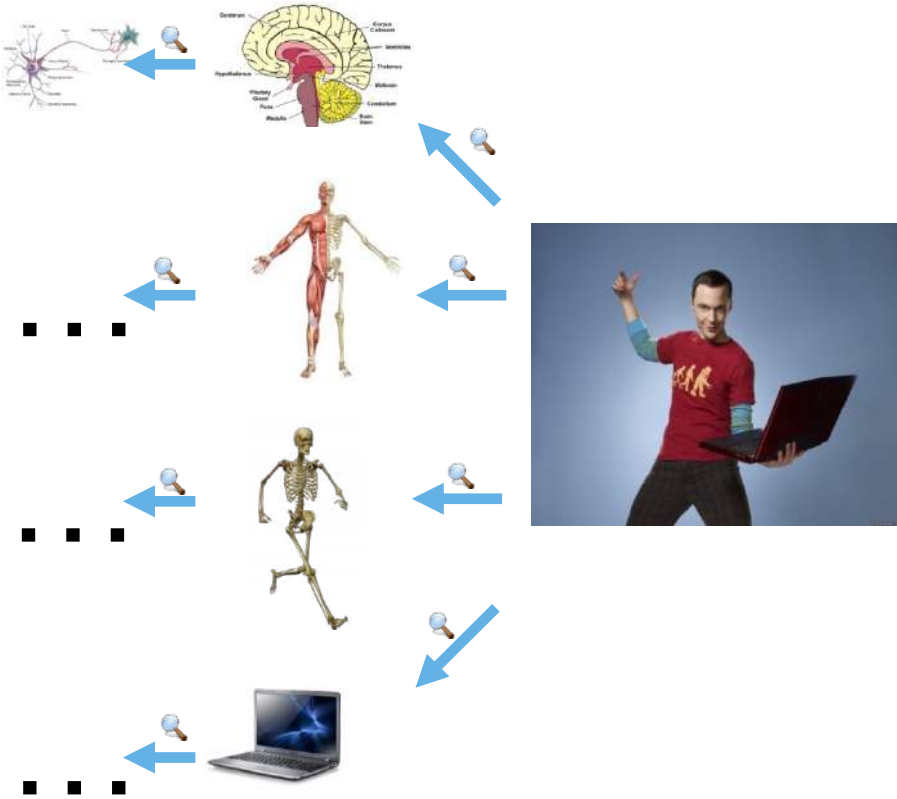
SCIENCE PARADIGMS

Reductionism



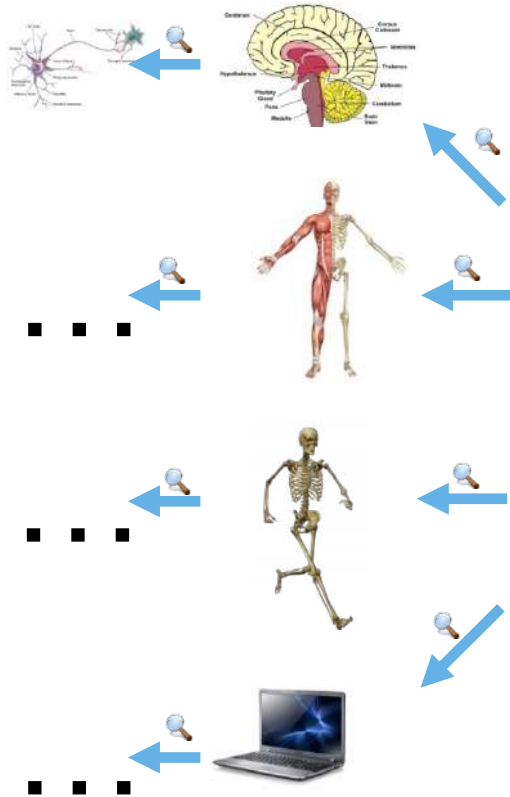
SCIENCE PARADIGMS

Reductionism

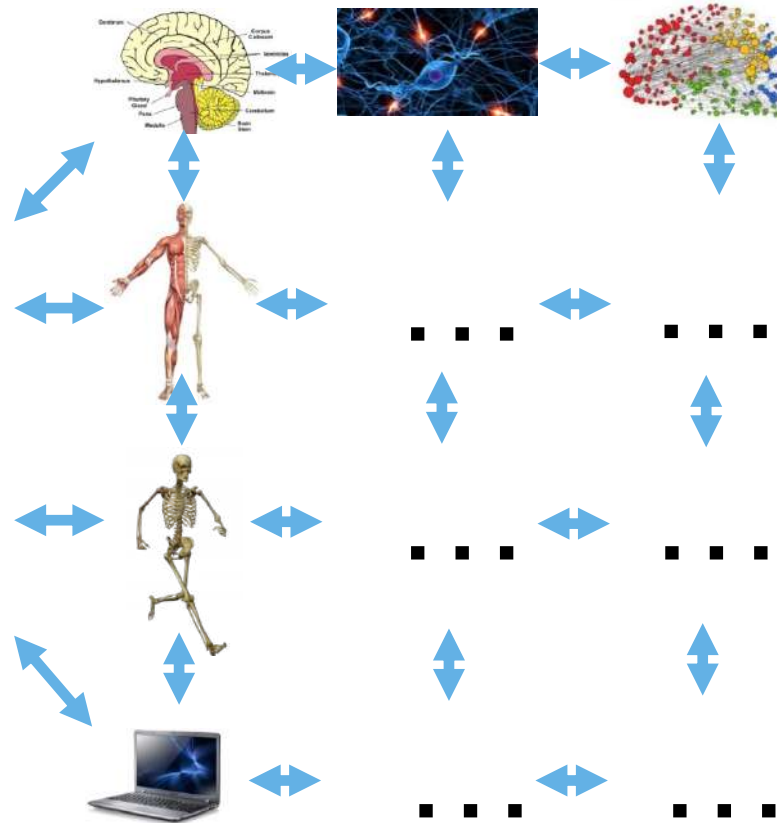


SCIENCE PARADIGMS

Reductionism

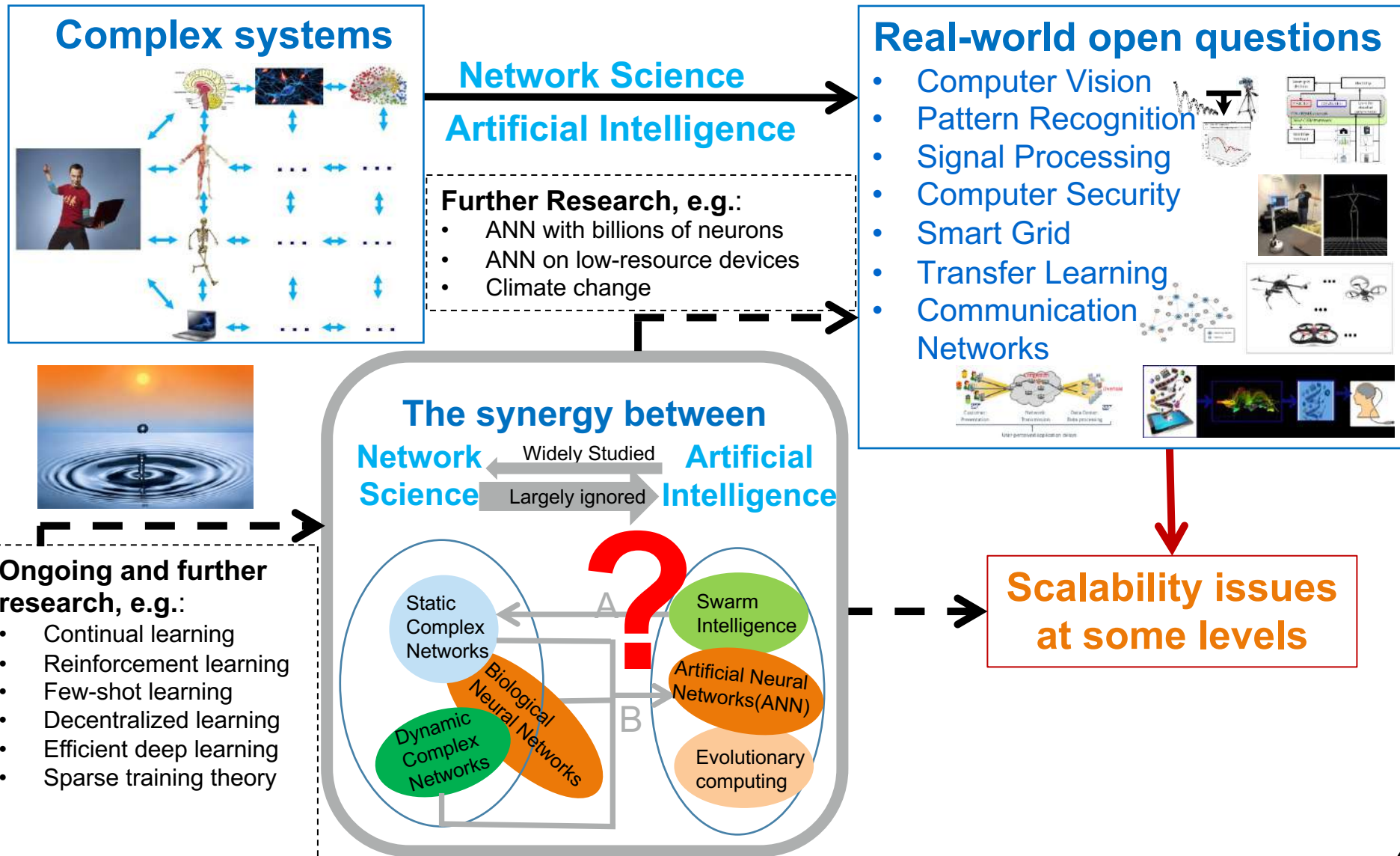


Complex Systems



*“the totality is not, as it were, a mere heap, but the whole is something beside the parts”, Aristotle, **Metaphysics**, ≈350 BC*

MY RESEARCH IN A NUTSHELL



References:

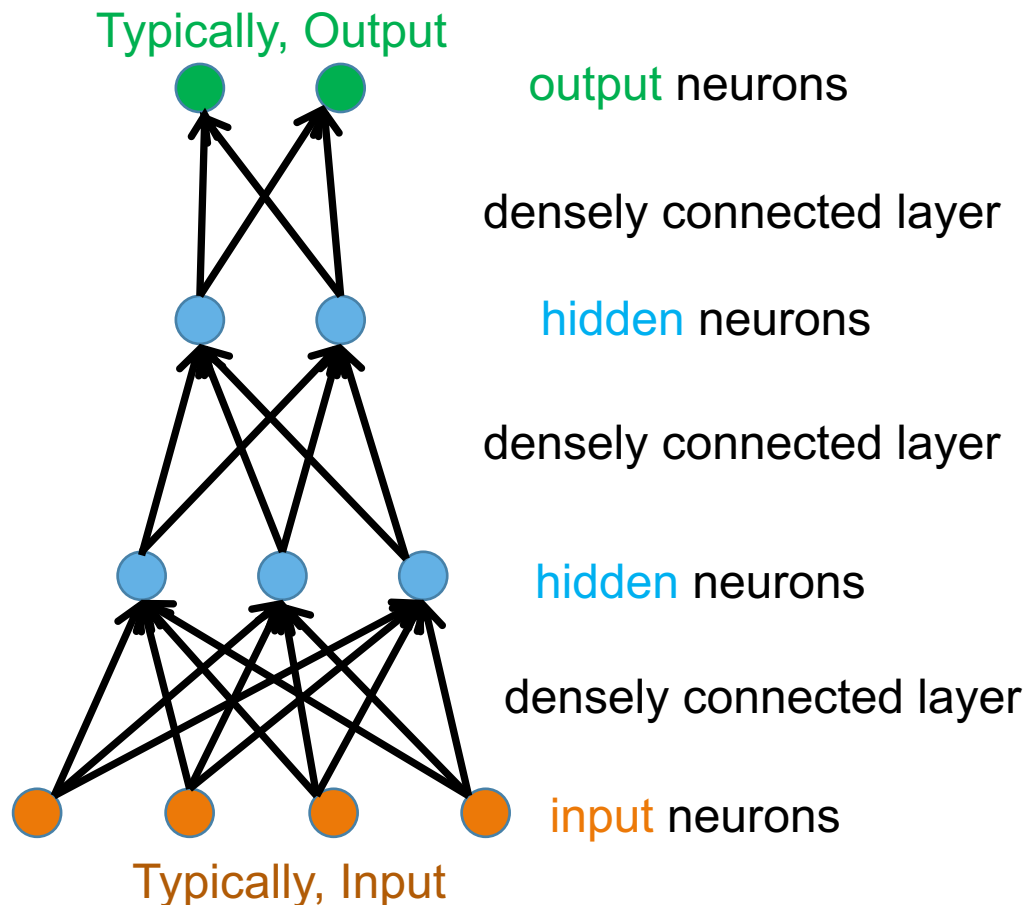
- D.C. Mocanu, *On the synergy of network science and artificial intelligence*, **IJCAI** 2016
- D.C. Mocanu, *Network computations in artificial intelligence*, **PhD thesis**, 2017
- [A] D.C. Mocanu, G. Exarchakos, A. Liotta, *Decentralized dynamic understanding of hidden relations in complex networks*, **Scientific Reports**, 2018
- [B] D.C. Mocanu, E. Mocanu, P. Stone, P.H. Nguyen, M. Gibescu, A. Liotta, *Scalable Training of Artificial Neural Networks with Adaptive Sparse Connectivity inspired by Network Science*, **Nature Communications**, 2018

ARTIFICIAL NEURAL NETWORKS (ANN)

BRIEF TECHNICAL BACKGROUND

Example of an ANN model
i.e., Multi Layer Perceptron (MLP)

"This model will be a simplification and an idealization, and consequently a falsification",
Alan Turing, 1952.



State-of-the-art (broadly speaking):

- ANN models are very good at single specialized tasks (e.g., recognizing cats) -> deep learning hype

RESEARCH AIMS

Long term: study the **synergy** between **network science** and **artificial intelligence** for the advancement of science and societal benefits.

Medium term:

- conceive **scalable** and **efficient** artificial **neural networks**
- capable to perform **continual (reinforcement) learning**
- and to **generalize** from limited multimodal data/experiences
- on **heterogeneous** known and unknown hierarchical **tasks**

Selected challenges for today talk:

1. **too many connections** to optimize in ANNs (due to densely connected layers); existing software and hardware is optimized just for dense neural networks - limiting their representational power, etc.
2. **catastrophic forgetting** (when learning new knowledge, an ANN model is prone to forget previously learnt knowledge)
3. and many other parts of a very large **puzzle** would have to be solved

...

MOTIVATION

Example of real-world problems



1200 pixels

1600 pixels 3 RGB channels
 $1600 \times 1200 \times 3 = 5.760.000$ dimensions

Biology:

- p53 Mutants Data Set
 - 5409 attributes
- Thrombin dataset
 - 139351 binary attributes
- Human chromosomes
 - Millions of attributes

Low-resources devices:



Extremely High Energy Consumption:

- For instance, GPT-3
 - 175 billion parameters
 - 355 GPU-years for training
 - 4.600.000 USD for training [Chuan Li, Lamdalabs, 2020]

State-of-the-art successful solutions and limitations

Deep Convolutional Neural Networks

- Work usually for images
- Usually still need some densely connected layers

Feature extraction/selection

- Needs expert knowledge of the field
- It is hard to automatize

Pruning methods – model compression

- They still need large densely connected layers
- Extremely high training time
- Models have to be trained in the cloud and after that have to be moved to the device

No solution (in practice) for the training phase

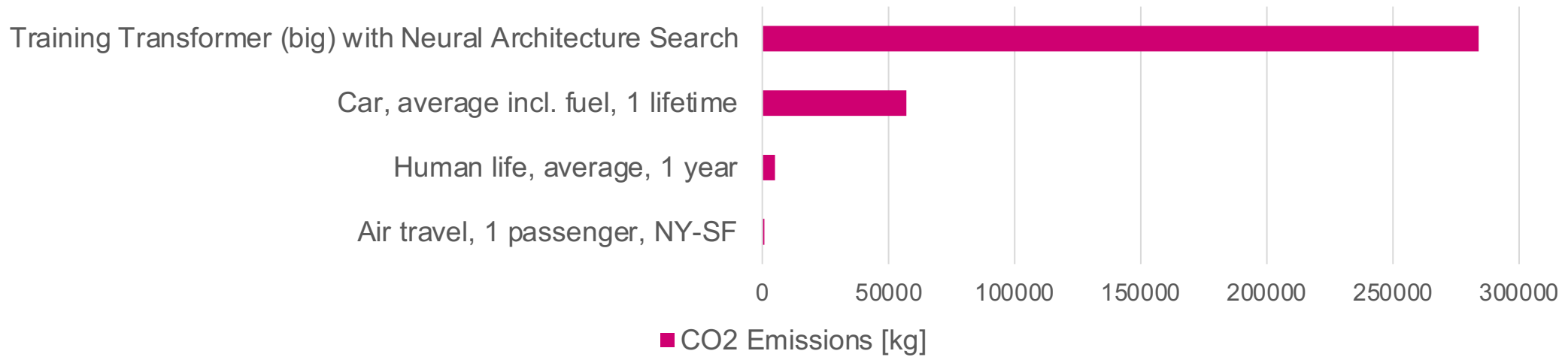
- Pruning for the exploitation phase

How to obtain scalable, performant, and efficient (deep) artificial neural networks?

- To handle better high dimensional data
- For faster computational time in training and exploitation (inference)

MOTIVATION

Carbon footprint comparison



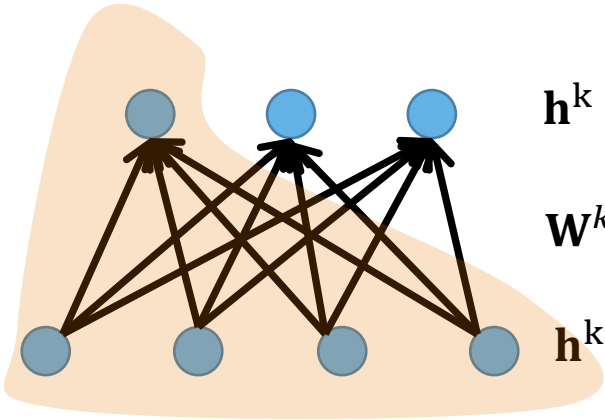
Reference:

- Emma Strubell, Ananya Ganesh, Andrew McCallum, *Energy and Policy Considerations for Deep Learning in NLP*, **ACL** 2019

BACKGROUND

Unnecessary connections in neural networks fully connected layers (problem)

Neural networks Fully-Connected (FC) k layer



$$\mathbf{h}^k = [h_1^k, h_2^k, \dots, h_{n^k}^k]$$

$$\mathbf{W}^k \in \mathbb{R}^{n^{k-1} \times n^k}$$

$$\mathbf{h}^{k-1} = [h_1^{k-1}, h_2^{k-1}, \dots, h_{n^{k-1}}^{k-1}]$$

Example of weights matrix (\mathbf{W}^k) after training

$$\mathbf{W}^k = \begin{pmatrix} 2 & 0.001 & 3 \\ -1 & -0.03 & 0.01 \\ 0.02 & -3 & -0.02 \\ 0.01 & 1.4 & 0.024 \end{pmatrix}$$

Weights close to zero don't count too much

$$h_1^k = f(h_1^{k-1}w_{11}^k + h_2^{k-1}w_{21}^k + h_3^{k-1}w_{31}^k + h_4^{k-1}w_{41}^k)$$

Problems with dense weights matrix:

- High computational time to optimize unnecessary weights
- High storage requirements to store unnecessary weights
- Unnecessary multiplications and additions

OUTLINE

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PRUNING

Schematic Procedure:

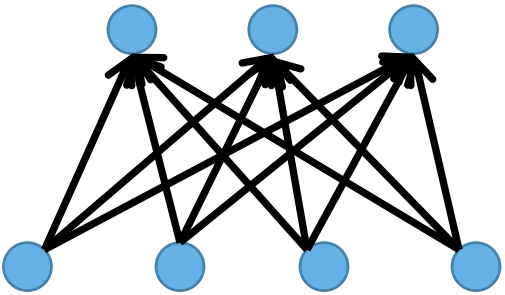
- *Step1*: Start with a fully-connected neural network
- *Step2*: Train the network until some convergence criteria is satisfied
- *Step3*: Identify unimportant connections based on some saliency criteria.
The most used in practice criteria are:
 - Magnitude (connections with values closed to zero)
 - Various information-theoretic criteria
- *Step4*: Prune those unimportant connections
- *Step5*: Repeat from *Step2* until the neural network satisfies the target trade-off sparsity/accuracy

PRUNING - A VISUAL EXAMPLE

Train the neural network until convergence is satisfied.

W^k after training

$$W^k = \begin{pmatrix} 2 & 0.001 & 3 \\ -1 & -0.03 & 0.01 \\ 0.02 & -3 & -0.02 \\ 0.01 & 1.4 & 0.024 \end{pmatrix}$$



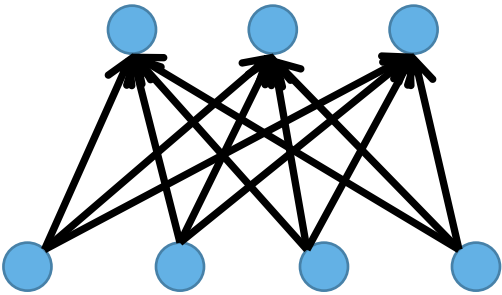
PRUNING - A VISUAL EXAMPLE

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W^k after training

$$W^k = \begin{pmatrix} 2 & 0.001 & 3 \\ -1 & -0.03 & 0.01 \\ 0.02 & -3 & -0.02 \\ 0.01 & 1.4 & 0.024 \end{pmatrix}$$

Use magnitude to identify unimportant connections.



PRUNING - A VISUAL EXAMPLE

Train the neural network until convergence is satisfied.

W^k after training

$$W^k = \begin{pmatrix} 2 & 0.001 & 3 \\ -1 & -0.03 & 0.01 \\ 0.02 & -3 & -0.02 \\ 0.01 & 1.4 & 0.024 \end{pmatrix}$$

Use magnitude to identify unimportant connections.

W^k after pruning

$$W^k = \begin{pmatrix} 2 & 0 & 3 \\ -1 & -0.03 & 0 \\ 0 & -3 & 0 \\ 0 & 1.4 & 0.024 \end{pmatrix}$$

Prune the unimportant connections.

Repeat until the neural network satisfies the target trade-off sparsity/accuracy.

REFERENCES

There is a considerable amount of work in the last years on this topic. Some are using magnitude and some are using various information metric criteria. It is almost impossible to cover all of it, and for this we apologize to many authors. Below are some references for further read.

Selected References:

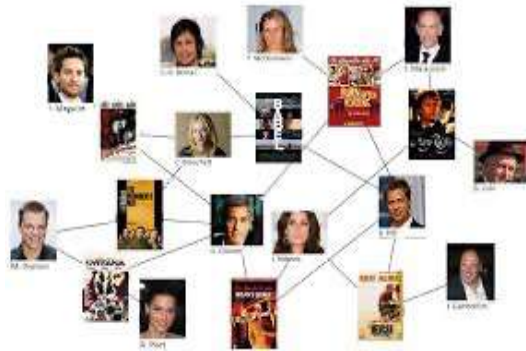
- Michael Mozer & Paul Smolensky. *Using Relevance to Reduce Network Size Automatically*. **Connection Science**, 1989.
- Yan Le Cun, John S. Denker, Sara A. Solla. *Optimal brain damage*. **NIPS**, 1990
- Babak Hassibi, David G. Stork. *Second order derivatives for network pruning: Optimal Brain Surgeon*. **NIPS**, 1993
- Song Han, Jeff Pool, John Tran, William J. Dally. *Learning both Weights and Connections for Efficient*, **NIPS**, 2015
- Dmitry Molchanov, Arsenii Ashukha, Dmitry Vetrov. *Variational Dropout Sparsifies Deep Neural Networks*, **ICML**, 2017

OUTLINE

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INSPIRATION

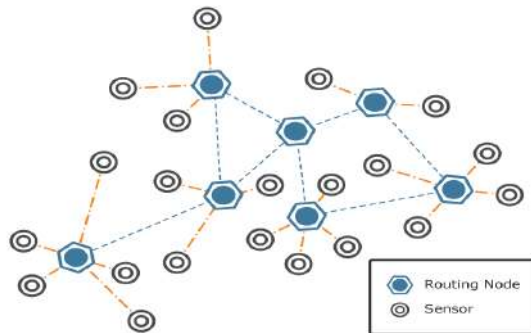
Social Networks



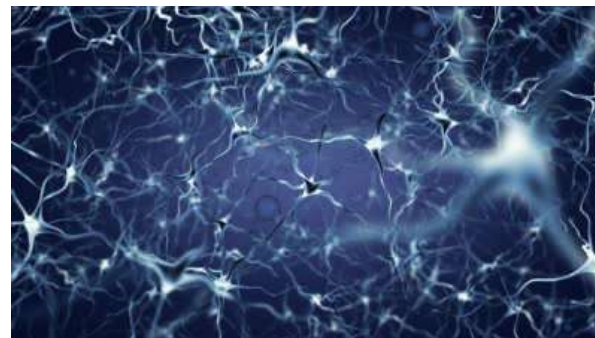
Transportation Networks



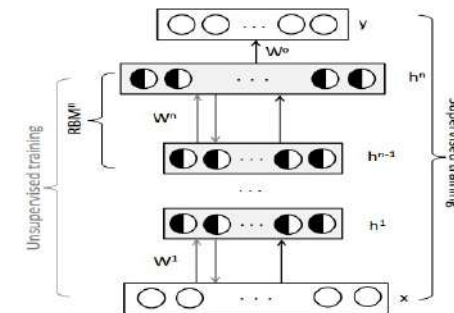
Wireless Sensors Networks



Biological Neural Networks



Artificial Neural Networks



INSPIRATION

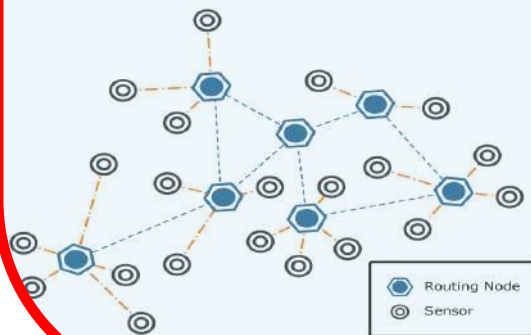
Social Networks



Transportation Networks



Wireless Sensors
Networks

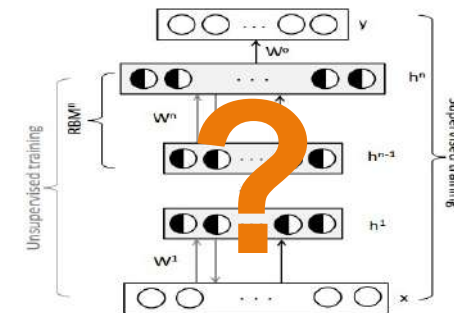


Biological Neural
Networks



Real world networks
are usually
intrinsically sparse
and evolve in time!

Artificial Neural Networks



PIECE 1 OF THE PUZZLE – PROPOSED CONCEPT ALWAYS SPARSE – NEVER DENSE

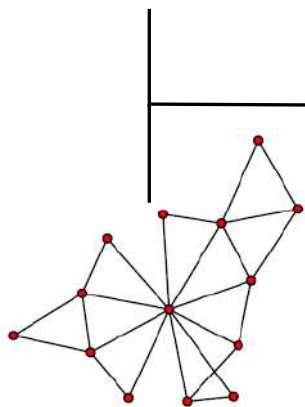
Our statements:

- ANN sparsity **must be** initiated from the design phase, **before training!!!!**

On par performance with dense training!

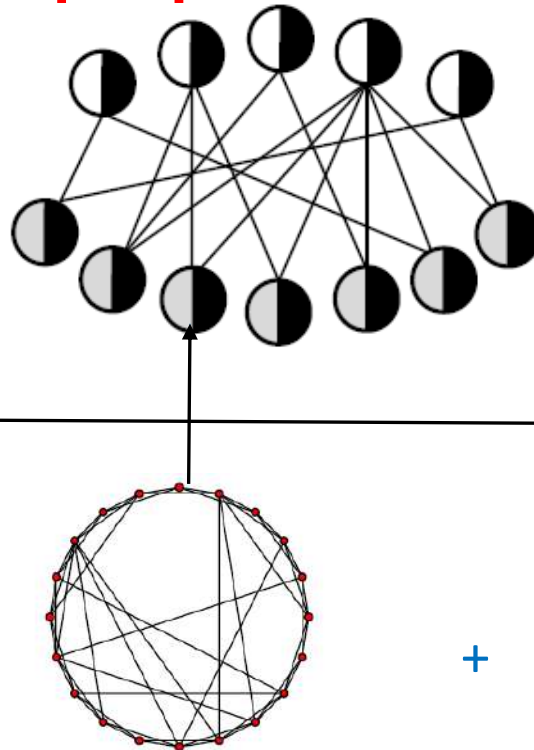


Data Statistics



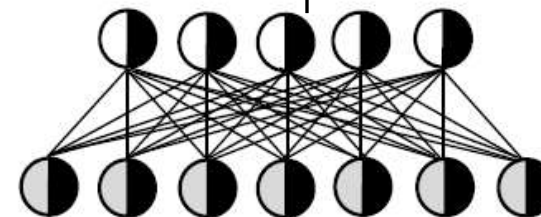
Scale-free topology

+



Small-world topology

+



Restricted Boltzmann machines

XBM

- sparse model
- static sparse connectivity
- fixed before training

References:

- D.C. Mocanu, E. Mocanu, P. Nguyen, M. Gibescu, A. Liotta, *A topological insight into restricted Boltzmann machines*, **Machine Learning Journal**, ECML-PKDD, 2016.

PIECE 1 OF THE PUZZLE – PROPOSED CONCEPT ALWAYS SPARSE – NEVER DENSE

Our statements:

- ANN **sparsity** **must be** initiated from the design phase, **before training!!!!**
- While training with **static sparse connectivity** leads to decent enough performance, **adaptive (dynamic) sparse connectivity** allows the model to properly fit the data and, consequently, to ensure higher performance!!!!

Adaptive sparse connectivity goal:

- Both, the connectivity graph and the connection weights, are optimized together during training!

References:

- D.C. Mocanu, E. Mocanu, P. Nguyen, M. Gibescu, A. Liotta, *A topological insight into restricted Boltzmann machines*, **Machine Learning Journal**, ECML-PKDD, 2016.
- D.C. Mocanu, *Network computations in artificial intelligence*, **PhD thesis**, 2017
- D.C. Mocanu, E. Mocanu, P. Stone, P.H. Nguyen, M. Gibescu, A. Liotta, *Scalable training of artificial neural networks with adaptive sparse connectivity inspired by network science*, arXiv:1707.04780, **Nature Communications**, 2018

PIECE 1 OF THE PUZZLE – PROPOSED SOLUTION

SPARSE EVOLUTIONARY TRAINING (SET)

SET – an efficient algorithm to train **sparsely connected layers** for ANNs with **adaptive sparse connectivity** which can safely replace any densely connected layer, at **no loss in accuracy**, while having **quadratically less parameters**. Thus:

- quadratically faster training time
- quadratically smaller memory footprint

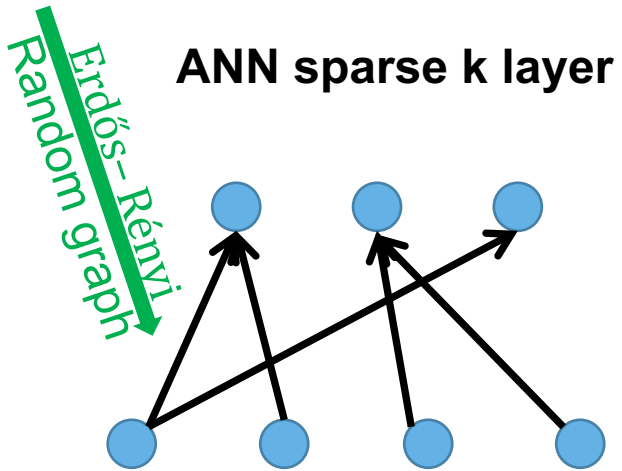
SET procedure:

- start with an Erdős–Rényi random graph topology for any bipartite layer:
 $p(w_{ij}^k) = \varepsilon(n^k + n^{k+1})/(n^k n^{k+1})$; ε – small integer, control sparsity level
- for each training epoch
 - perform standard training procedure;
 - for each bipartite layer:
 - remove a fraction ζ of the smallest positive weights;
 - remove a fraction ζ of the largest negative weights;
 - add randomly new weights (connections) in the same amount as the ones removed previously

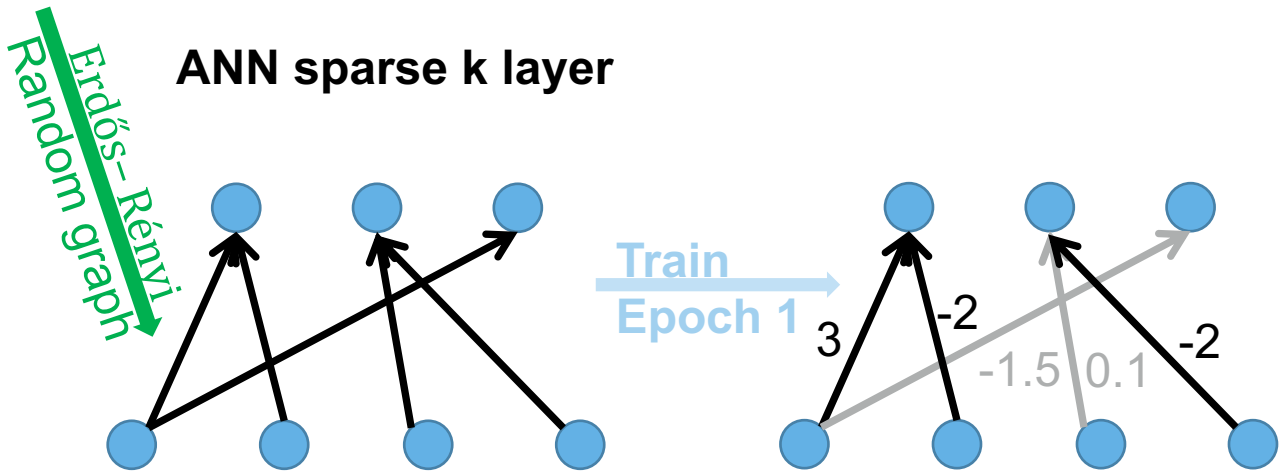
References:

- D.C. Mocanu, *Network computations in artificial intelligence*, **PhD thesis**, 2017
- D.C. Mocanu, E. Mocanu, P. Stone, P.H. Nguyen, M. Gibescu, A. Liotta: *Scalable training of artificial neural networks with adaptive sparse connectivity inspired by network science*, arXiv:1707.04780, **Nature Communications**, 2018

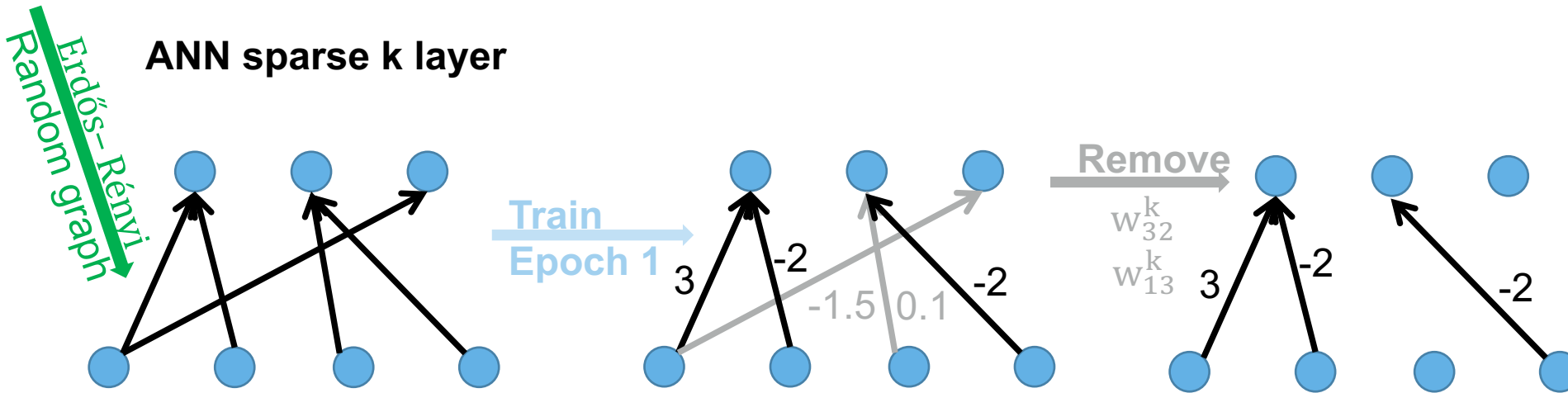
PIECE 1 OF THE PUZZLE – MECHANISM SPARSE EVOLUTIONARY TRAINING (SET)



PIECE 1 OF THE PUZZLE – MECHANISM SPARSE EVOLUTIONARY TRAINING (SET)

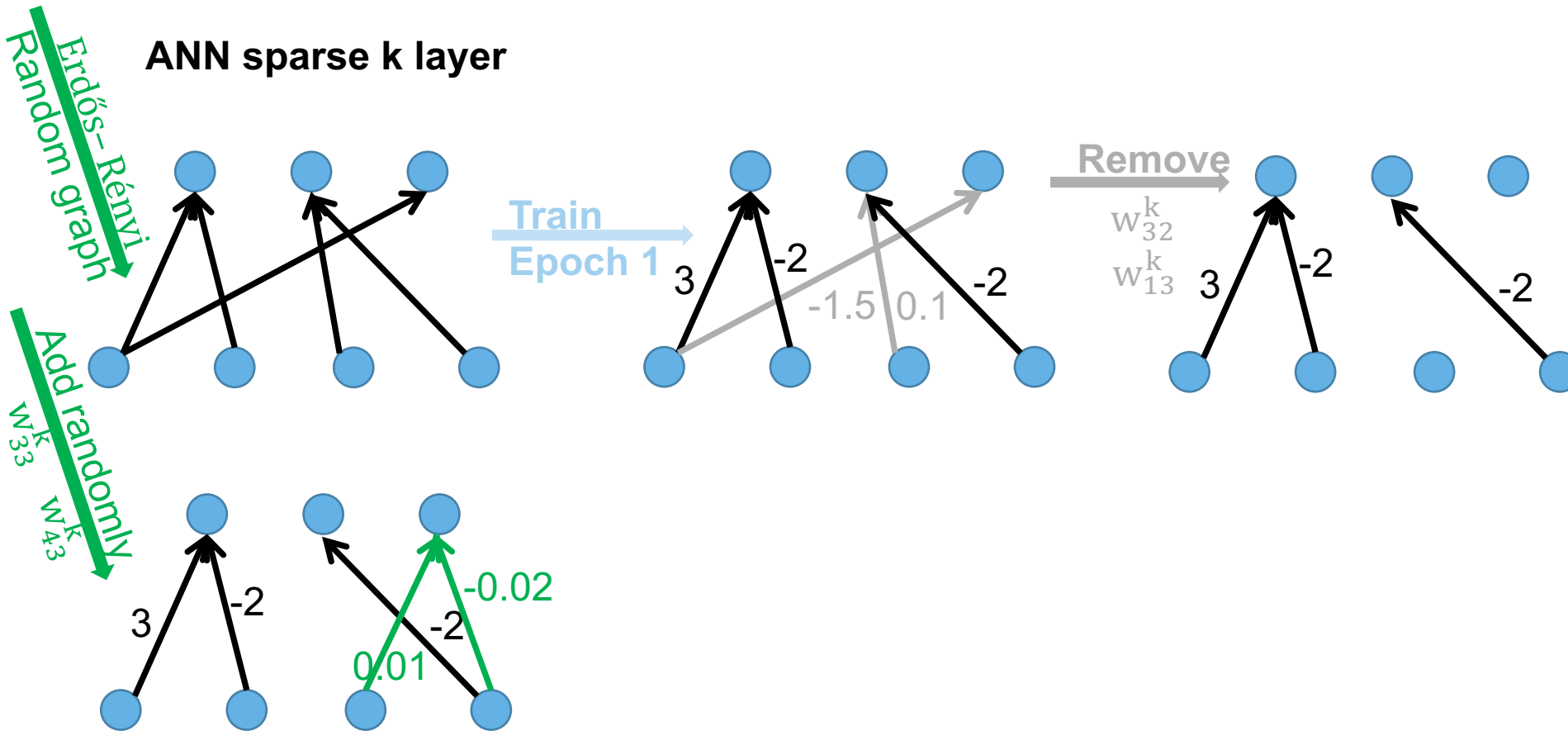


PIECE 1 OF THE PUZZLE – MECHANISM SPARSE EVOLUTIONARY TRAINING (SET)



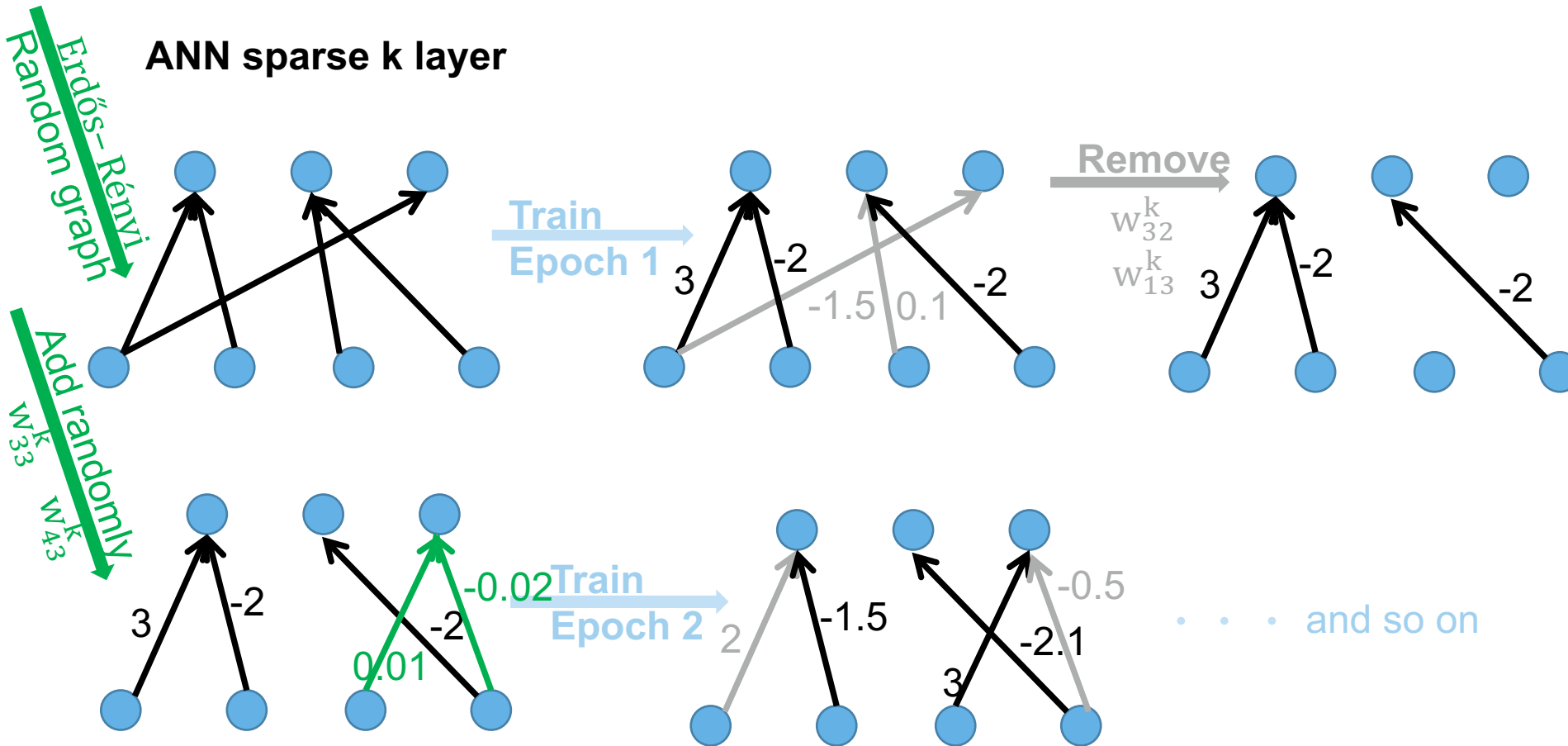
PIECE 1 OF THE PUZZLE – MECHANISM

SPARSE EVOLUTIONARY TRAINING (SET)



PIECE 1 OF THE PUZZLE – MECHANISM

SPARSE EVOLUTIONARY TRAINING (SET)



PIECE 1 OF THE PUZZLE

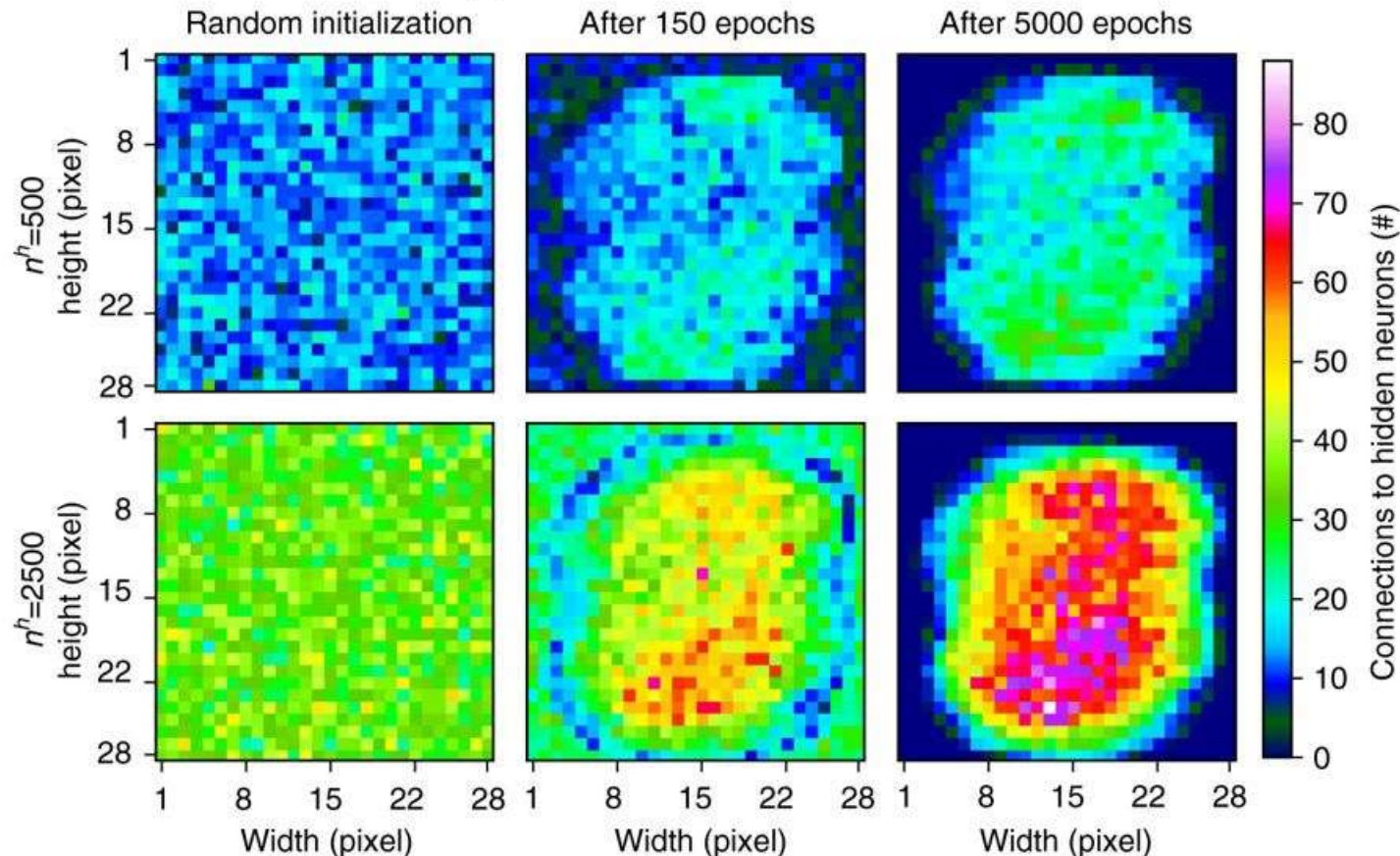
SET – AUTOMATIC PATTERN DISCOVERY

a

Examples of images from MNIST dataset



Connectivity patterns of the visible neurons of a SET-RBM

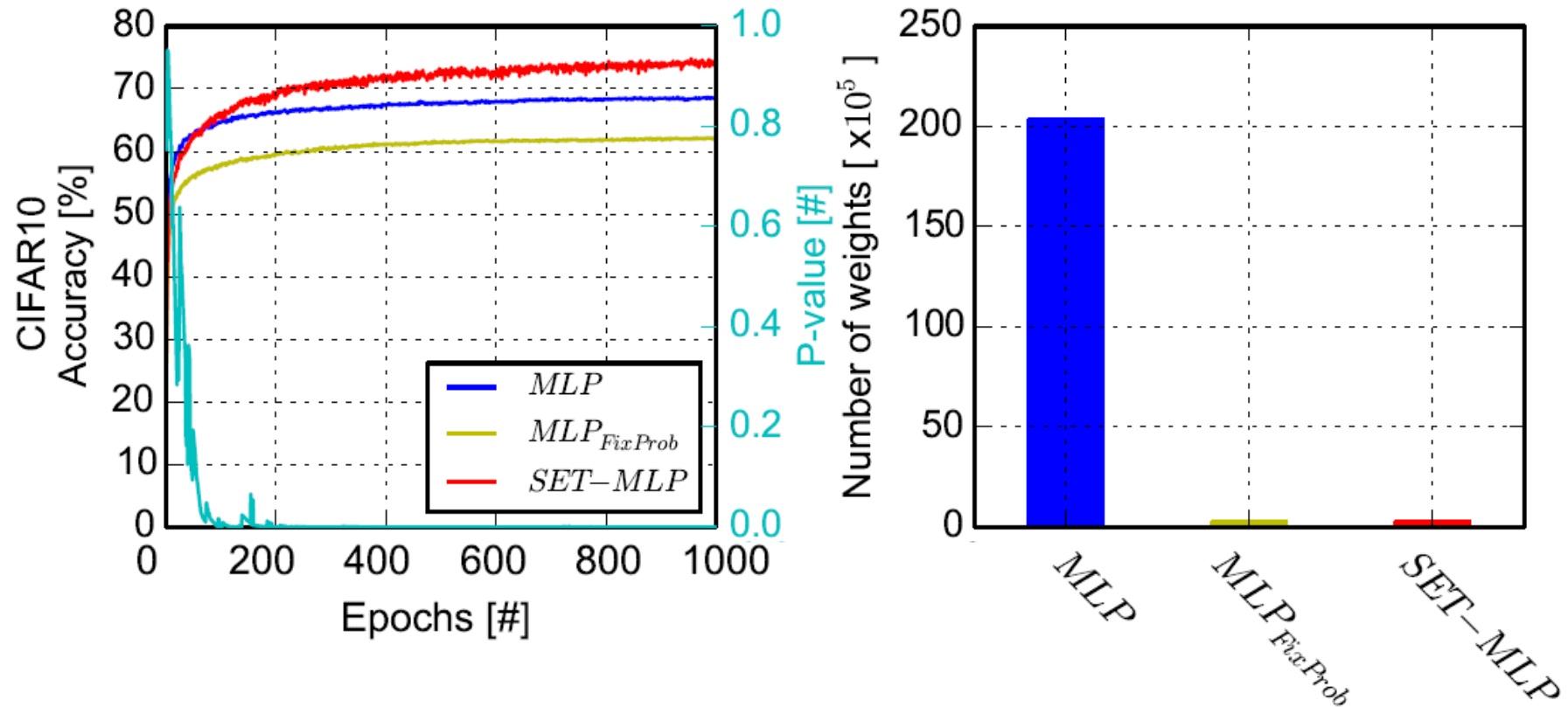


References:

- D.C. Mocanu, E. Mocanu, P. Stone, P.H. Nguyen, M. Gibescu, A. Liotta, *Scalable training of artificial neural networks with adaptive sparse connectivity inspired by network science*, arXiv:1707.04780, **Nature Communications**, 2018

PIECE 1 OF THE PUZZLE

SET – SUPERVISED LEARNING

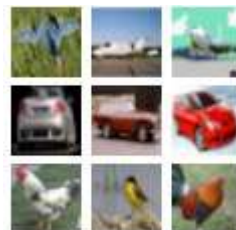


Reference:

- D.C. Mocanu, E. Mocanu, P. Stone, P.H. Nguyen, M. Gibescu, A. Liotta, *Scalable training of artificial neural networks with adaptive sparse connectivity inspired by network science*, arXiv:1707.04780, **Nature Communications**, 2018

Dataset:

- CIFAR 10 (object recognition)
- 10 classes



PIECE 1 OF THE PUZZLE – INTERMEZZO

Impact: SET (Sparse Evolutionary Training) put the basis of the emerging subfield of (Dynamic) Sparse Training.

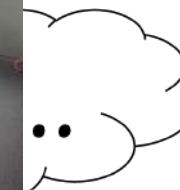


D.C. Mocanu, E. Mocanu, Z. Vale, D. Ernst, *Scalable Deep Learning* (T24), tutorial at **International Joint Conference on Artificial Intelligence**



S. Liu, G. Sokar, Z. Atashgahi, D.C. Mocanu, E. Mocanu, *Sparse Neural Networks Training*, tutorial at **ECMLPKDD 2022** ☺

Mocanu, T. Pinto, Z. Vale, *Scalable Deep Learning: how far is one billion* International Joint Conference on Artificial Intelligence (IJCAI), 2020.



...pandemic times ...

OUTLINE

- Context&Motivation
- Dense-to-sparse training
- *Sparse-to-sparse training*
 - principles
 - *utilization*

PIECE 1 OF THE PUZZLE

TRULY SPARSE IMPLEMENTATIONS

ONE MILLION NEURONS ON A LAPTOP WITHOUT GPU

Microarray gene expression data:

- very high dimensionality
- small number of samples
- e.g., Leukemia dataset (54,675 features, 2096 samples, 18 classes)
- traditional approach (feature selection/extraction + classifier)

Reference:

- Shiwei Liu, Decebal Constantin Mocanu, Amarsagar Reddy Ramapuram Matavalam, Yulong Pei, Mykola Pechenizkiy, *Sparse evolutionary Deep Learning with over one million artificial neurons on commodity hardware*, arXiv:1901.09181, **Neural Computing and Applications**, 2021

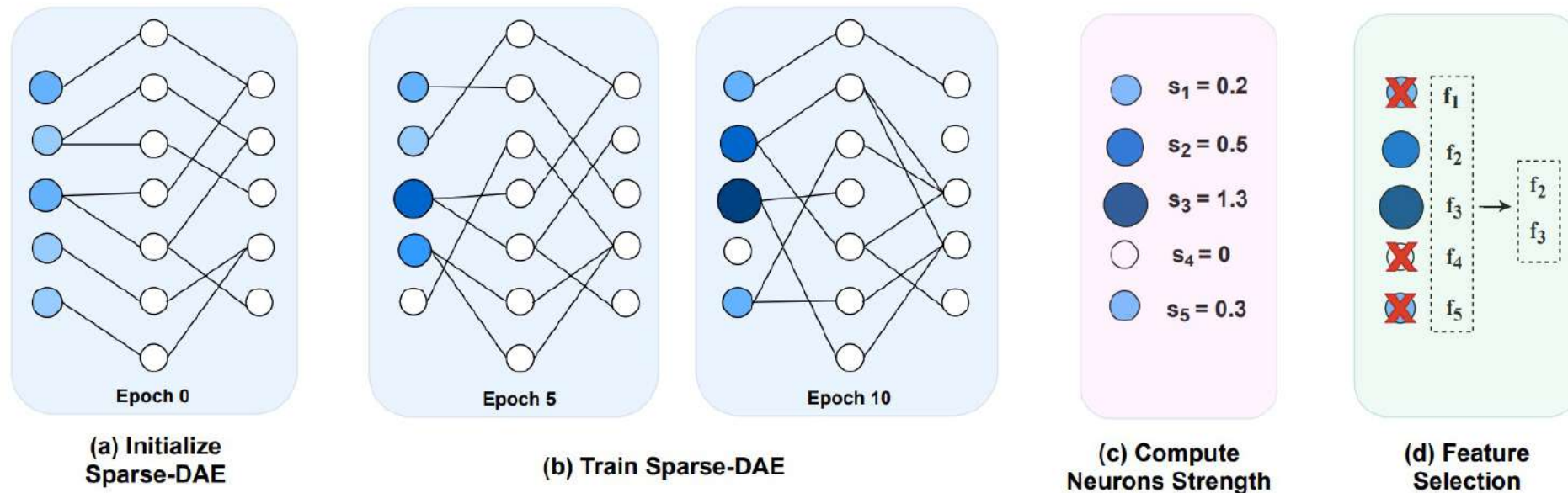
Model	Hardware	Density level (%)	Total time (s) (train + test)	Accuracy (%)
Small SET-MLP	1 CPU thread	1.04	65	82.88 ± 1.18
Large SET-MLP	1 CPU thread	0.007	4914	81.83 ± 1.11
mrPSVM [40]	Conventional	n/a	1265	81.1
mrPSVM [40]	Hadoop cluster	n/a	291	81.1

- mrPSVM (ensemble of feature selection algorithms + support vector machine) from Kumar M, Rath SK (2015) *Classification of microarray using mapreduce based proximal support vector machine classifier*, **Knowl Based Syst** 89:584–602

PIECE 1 OF THE PUZZLE

QUICKSELECTION (QS)

DYNAMIC SPARSE TRAINING FOR UNSUPERVISED FEATURE SELECTION



DAE: Denoising Autoencoder

Neuron Strength:
$$s_i = \sum_{j=1}^{n^1} |W_{ij}^1|$$

References:

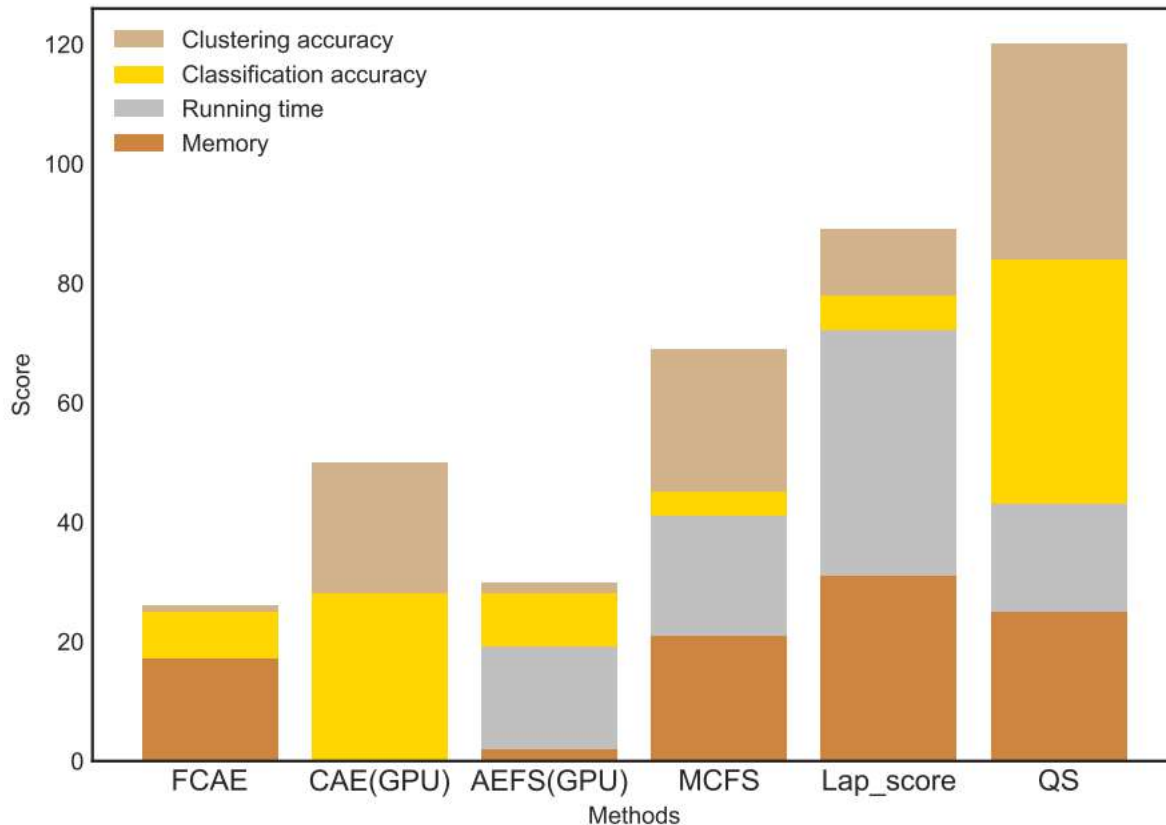
- Zahra Atashgahi, Ghada Sokar, Tim van der Lee, Elena Mocanu, Decebal Constantin Mocanu, Raymond Veldhuis, Mykola Pechenizkiy, *Quick and Robust Feature Selection: the Strength of Energy-efficient Sparse Training for Autoencoders*, **Machine Learning journal**, ECML-PKDD 2022

PIECE 1 OF THE PUZZLE

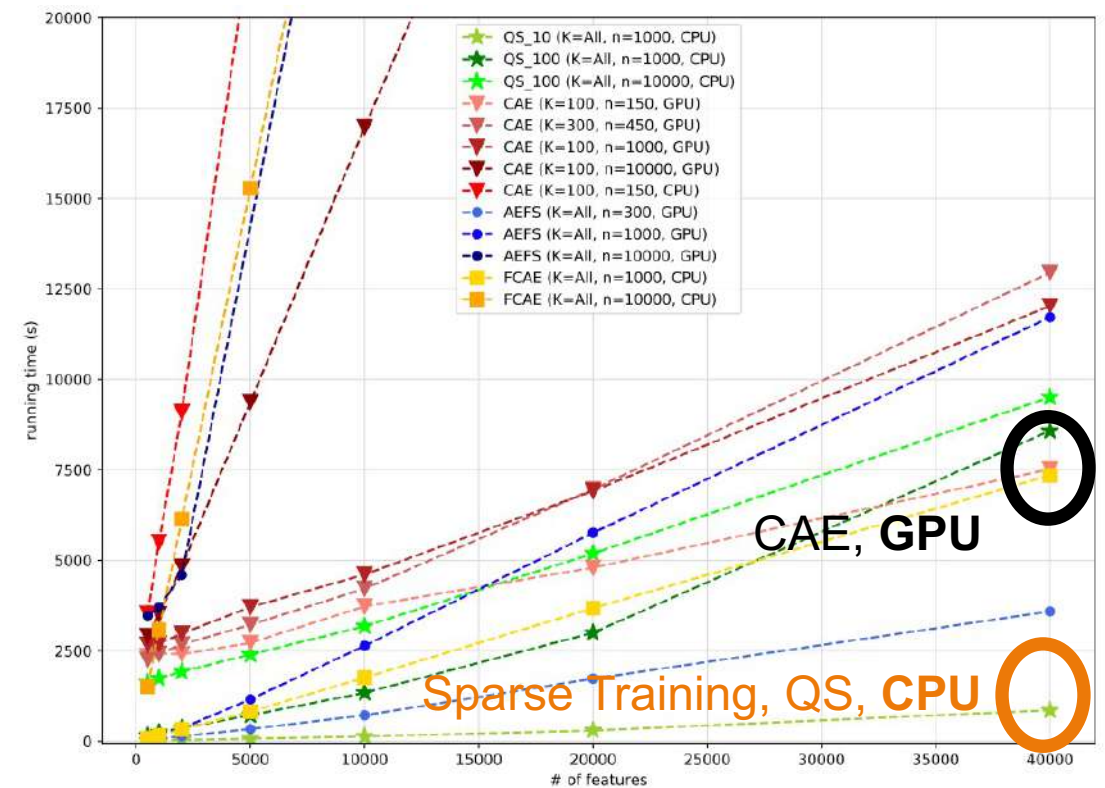
QUICKSELECTION (QS)

DYNAMIC SPARSE TRAINING FOR UNSUPERVISED FEATURE SELECTION

Results summary (over 8 datasets, ranked 1st or 2nd)



Artificial dataset – running time



References:

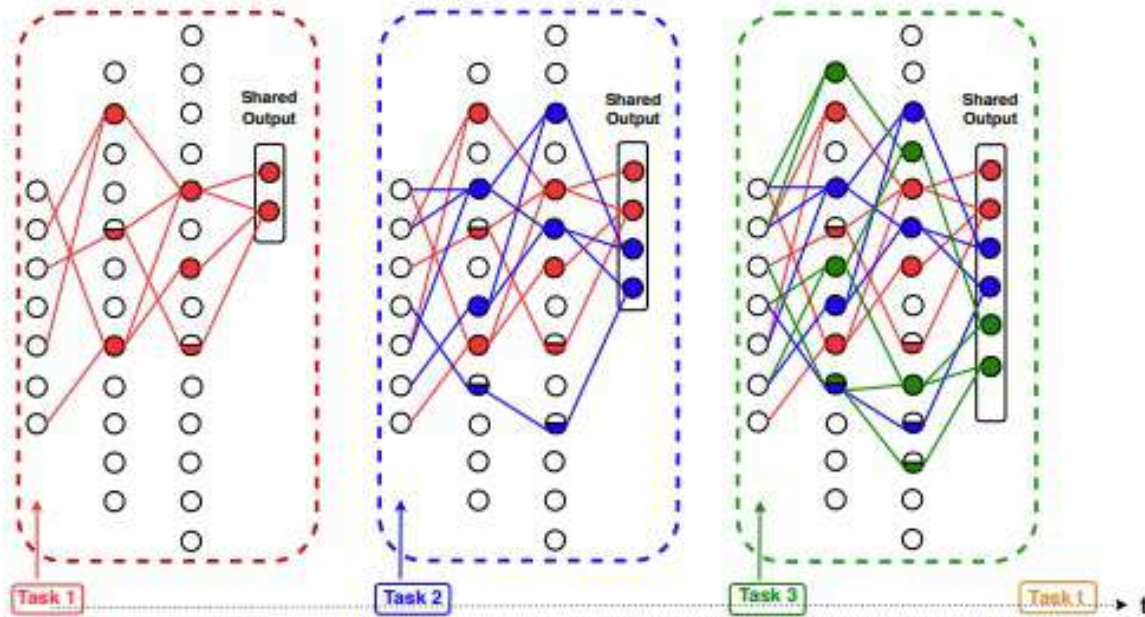
- Zahra Atashgahi, Ghada Sokar, Tim van der Lee, Elena Mocanu, Decebal Constantin Mocanu, Raymond Veldhuis, Mykola Pechenizkiy, *Quick and Robust Feature Selection: the Strength of Energy-efficient Sparse Training for Autoencoders*, **Machine Learning journal**, ECML-PKDD 2022

PIECE 1 AND 2 OF THE PUZZLE

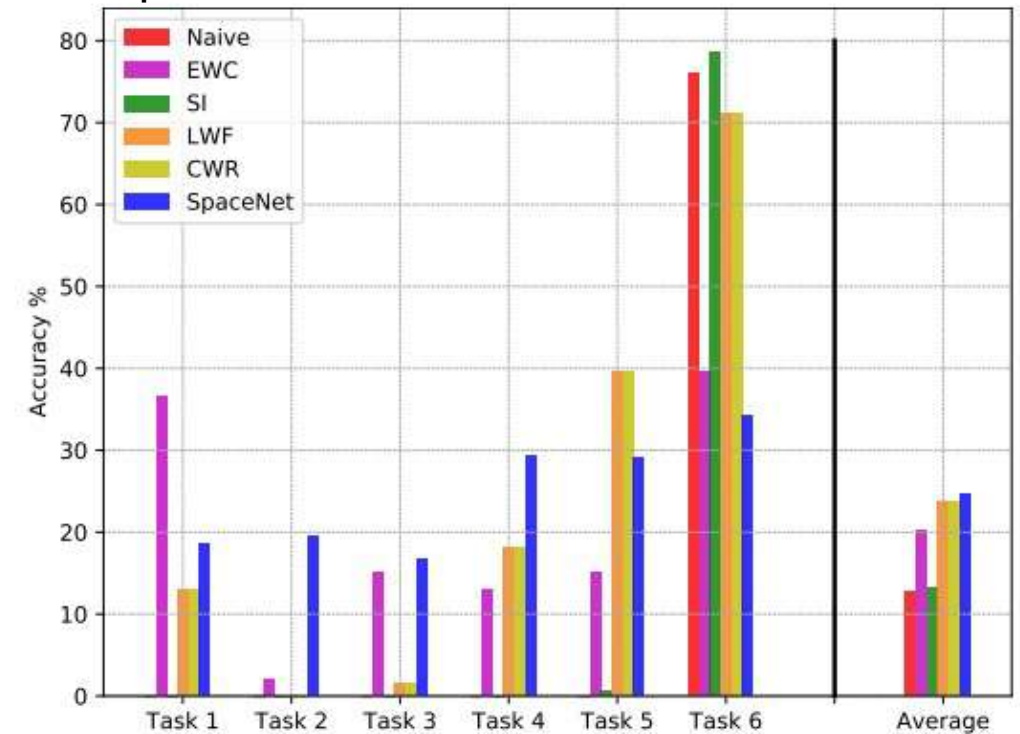
SPACENET

SPARSE TRAINING AND CONTINUAL LEARNING

SpaceNet schematic architecture



SpaceNet results on CIFAR 10/100



Reference:

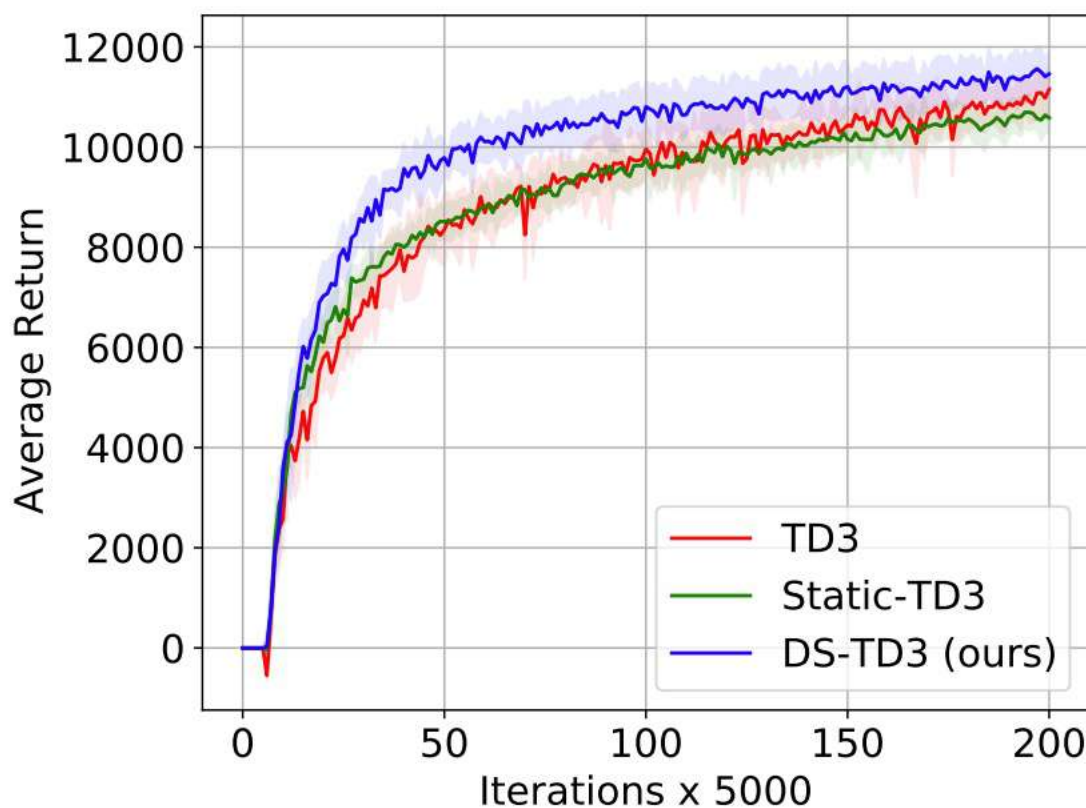
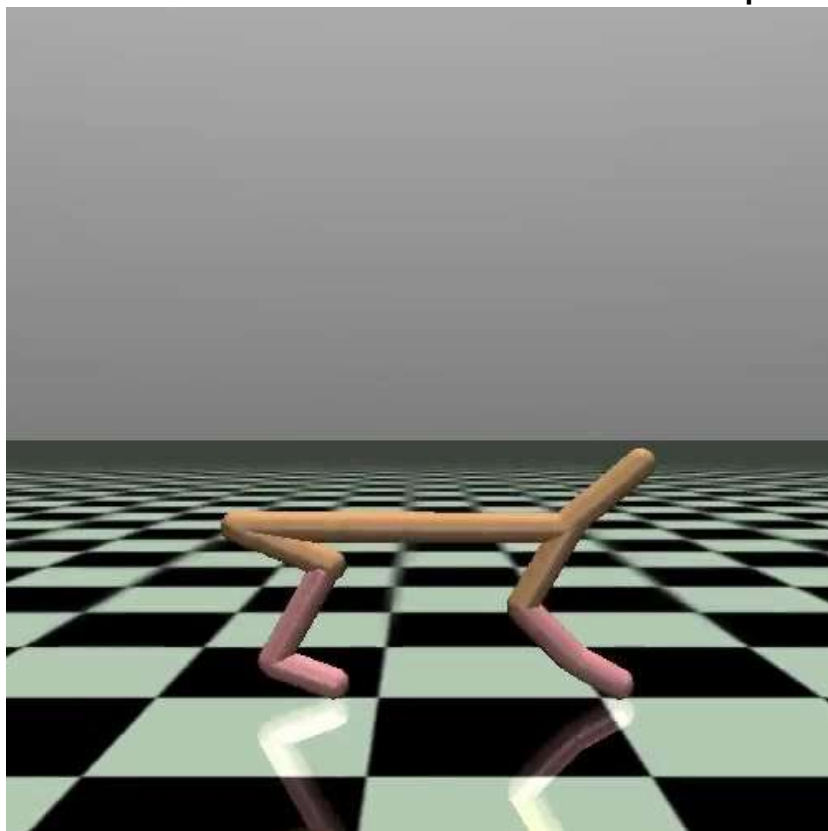
- Ghada Sokar, Decebal Mocanu, Mykola Pechenizkiy, *SpaceNet: Make Free Space For Continual Learning*, arXiv:2007.07617 (2020), **Neurocomputing**, 2021

PIECE 1 OF THE PUZZLE

DYNAMIC SPARSE TD3 (DS-TD3)

SPARSE TRAINING AND DEEP REINFORCEMENT LEARNING

Continuous control tasks with sparse MLPs optimized by sparse training. An example on Half Cheetah.



dense connectivity

static sparse connectivity

adaptive sparse connectivity
(50% sparsity level)

Reference:

- Ghada Sokar, Elena Mocanu, Decebal Constantin Mocanu, Mykola Pechenizkiy, Peter Stone, *Dynamic sparse training for deep reinforcement learning*, arXiv:2106.04217, IJCAI 2022, (and best paper award at AAMAS 2022 - ALA workshop)

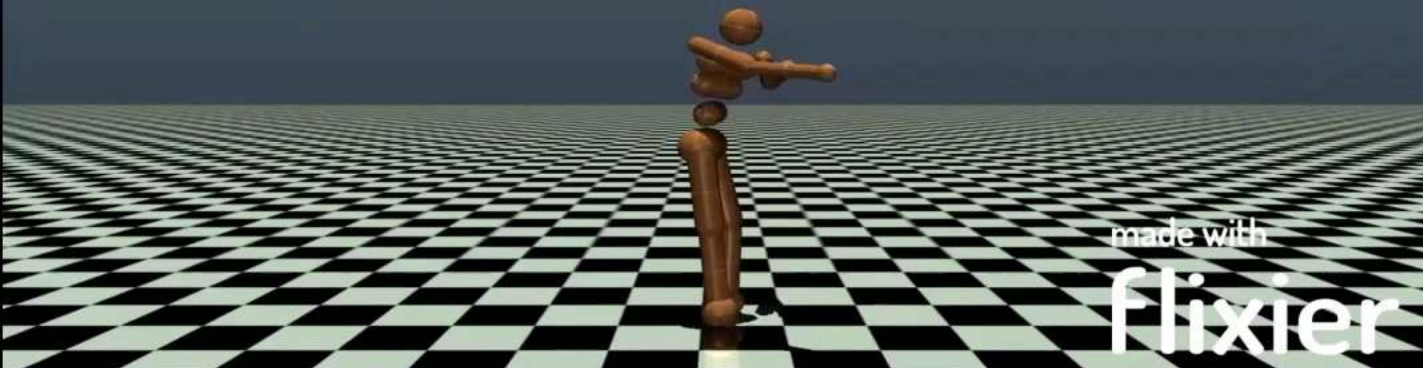
Algorithm: DS-TD3
Return: 72.40
Training Steps: 430000

Dynamic Sparse TD3



Algorithm: TD3
Return: 502.46
Training Steps: 430000

TD3



PIECE 1 OF THE PUZZLE SPARSE TRAINING AND DEEP REINFORCEMENT LEARNING

Reference:

- Ghada Sokar, Elena Mocanu, Decebal Constantin Mocanu, Mykola Pechenizkiy, Peter Stone, *Dynamic sparse training for deep reinforcement learning*, arXiv:2106.04217, **IJCAI 2022**, (and best paper award at AAMAS 2022 - **ALA** workshop)

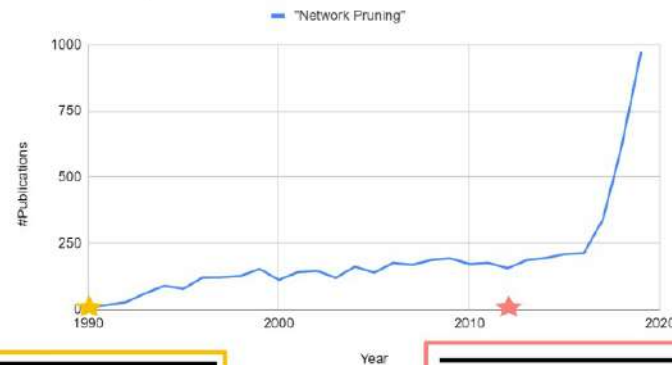
PIECE 1 OF THE PUZZLE

SPARSE TRAINING – CHALLENGES AND FUTURE

- Deep learning hardware and software is optimized for dense matrices (main challenge)
- Sparse training behaviour is not fully understood yet

The situation is changing - NVIDIA A100 GPU (released in 2020) supports 2:4 sparsity

Publications per Year



Reference:

- Jeff Pool, *Accelerating sparsity in NVIDIA ampere architecture*, 2020

Optimal Brain Damage

Yann Le Cun, John S. Denker and Sara A. Solla
AT&T Bell Laboratories, Holmdel, N. J. 07733

ImageNet Classification with Deep Convolutional Neural Networks

Alex Krizhevsky Ilya Sutskever Geoffrey E. Hinton
University of Toronto University of Toronto University of Toronto
krizhe@cs.utoronto.ca ilya@cs.utoronto.ca hinton@cs.utoronto.ca

Would you like to know more?

ICLR SNN 2023 Workshop, 5 May, hybrid, Kigali, Rwanda.

(Sparsity in Neural Networks: On practical limitations and tradeoffs between sustainability and efficiency)

<https://www.sparseneural.net/>

PIECE 1 OF THE PUZZLE

SPARSE TRAINING – SUPPLEMENTARY REFERENCES

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- [Reinforcement Learning] Laura Graesser, Utku Evci, Erich Elsen, Pablo Samuel Castro, *The State of Sparse Training in Deep Reinforcement Learning*, **ICML** 2022
- [Continual Learning] Ghada Sokar, Decebal C. Mocanu, and Mykola Pechenizkiy, *Avoiding Forgetting and Allowing Forward Transfer in Continual Learning via Sparse Networks*, **ECMLPKDD** 2022
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PIECE 1 OF THE PUZZLE

SPARSE TRAINING – OPEN-SOURCE CODE EXAMPLES

From our team

Simulating sparsity with binary masks

- <https://github.com/dcmocanu/sparse-evolutionary-artificial-neural-networks>
- <https://github.com/Shiweiliu11111111/In-Time-Over-Parameterization>
- <https://github.com/VITA-Group/FreeTickets>
- https://github.com/VITA-Group/Random_Pruning
- <https://github.com/zahraatashgahi/CTRE>
- <https://github.com/QiaoXiao7282/DSN>

Truly sparse implementations:

- <https://github.com/dcmocanu/sparse-evolutionary-artificial-neural-networks>
- <https://github.com/SelimaC/large-scale-sparse-neural-networks>

Sparse neural networks understanding:

- https://github.com/Shiweiliu11111111/Sparse_Topology_Distance

Feature selection with truly sparse implementation:

- <https://github.com/zahraatashgahi/QuickSelection>

For continual learning

- <https://github.com/GhadaSokar/SpaceNet>
- <https://github.com/GhadaSokar/AFAF>

For deep reinforcement learning

- <https://github.com/GhadaSokar/Dynamic-Sparse-Training-for-Deep-Reinforcement-Learning>
- <https://github.com/bramgrooten/automatic-noise-filtering>

From the community

Simulating sparsity with binary mask

- <https://github.com/IntelAI/dynamic-reparameterization>
- https://github.com/TimDettmers/sparse_learning
- <https://github.com/google-research/rigl>
- <https://github.com/boone891214/MEST>

FUTURE AIMS

These are difficult challenges. There is hard work ahead of us!

- ✓ for all common dense ANN architectures:
 - corresponding sparse ANNs
 - truly sparse software framework
- ❖ over 10x energy consumption and costs reduction
- ❖ over 10x reduction in CO₂ deep learning emissions
- ❖ enabling ANN training at the edge
- ✓ formal basis of sparse training theory:
 - increased performance
 - understanding
 - trust
- ❖ increased user confidence for sensitive tasks
- ❖ push AI knowledge well beyond state-of-the-art
- ❖ ANN paradigm shift
- ✓ novel sparse ANN architectures:
 - efficiency
 - decentralization
 - self-organization
 - native parallelism
- ❖ enabling realistic continual learning
- ❖ enabling ANNs to address very complex problems
- ❖ enabling ANNs with billions of neurons

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