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IPARCOS



UNIVERSIDAD
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MADRID

ERC Project

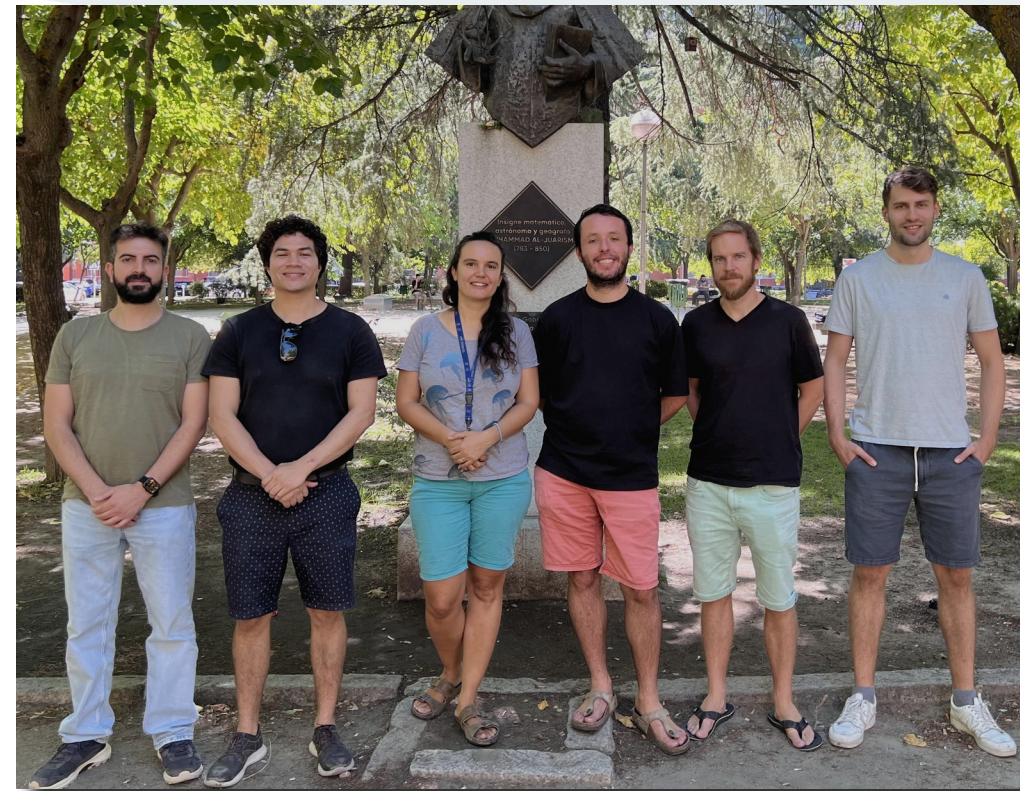
Beyond Maximum Entropy: *A new paradigm for Modeling, Inference, and Learning Efficiency*

IPARCOS Scientific Advisory Board: Bi-Annual Review 2026

Group's Overview

Group Snapshot

- **Physics of Machine Learning**, PIs Aurélien Decelle (UPM) & Beatriz Seoane (UCM)
- **Current Size:** Total members (2 Staff, 2 PhD, 4 Master, 2 visiting).
- **Key Personnel Changes:** 1 postdoc left, **new hirings 2026:** 3 postdocs + 1PhD



Key Performance Indicators

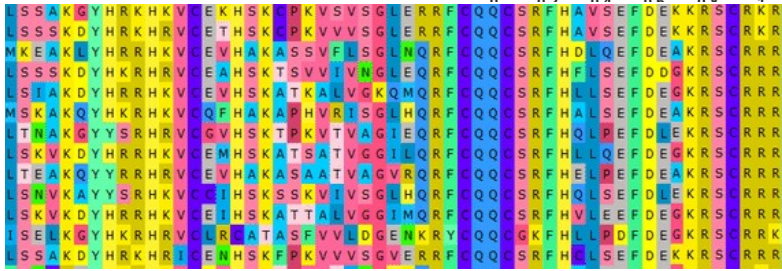
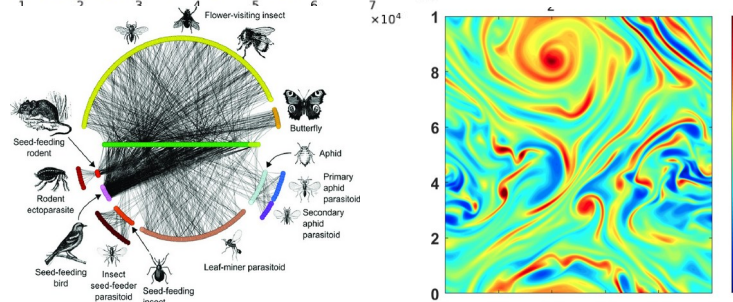
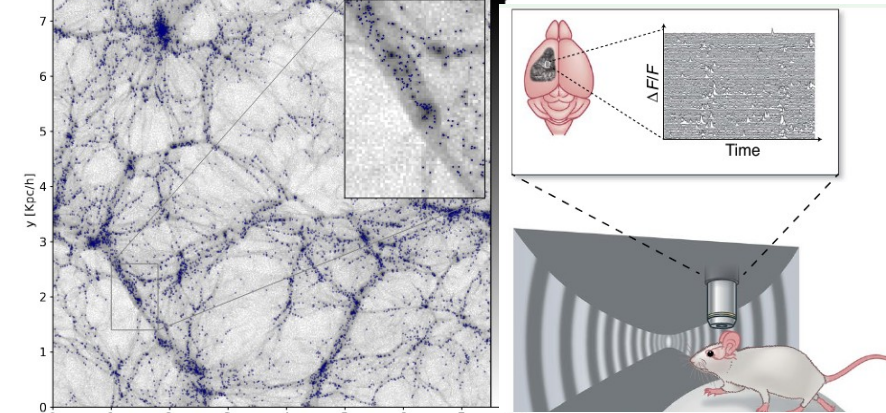
- **High-Impact Publications:** 15 peer-reviewed papers (10 in Q1 with 5 in D1 journals, 3 in A* conferences CS)
- **Funding Secured:** Consolidator ERC grant (2025), PID2024-158623NB-C21 (Coordinated project with the BIFI)
- **Training:** 2-PhD ongoing, one defending in 2026



Goal: Modeling scientific data

Dataset $\mathcal{D} = \{ \mathbf{x}^{(m)} \}_{m=1}^M$ $p_{\text{data}}(\mathbf{x}) = \frac{1}{M} \sum_{m=0}^M \delta(\mathbf{x} - \mathbf{x}^{(m)})$

$p_{\text{data}}(\mathbf{x}) \sim p_{\theta}(\mathbf{x})$



| id | gender | age | hypertension | heart_disease | ever_married | work_type | Residence_type | avg_glucose_level | bmi | smoking_status | stroke | |
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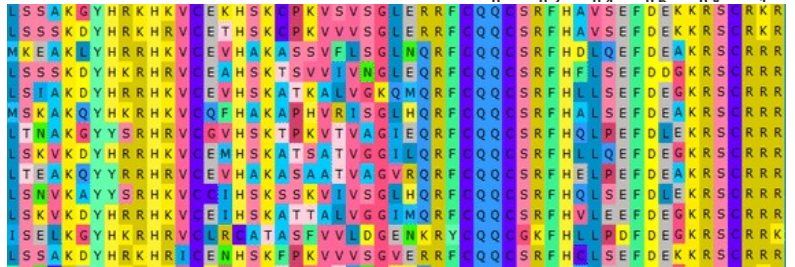
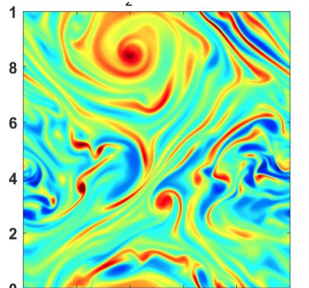
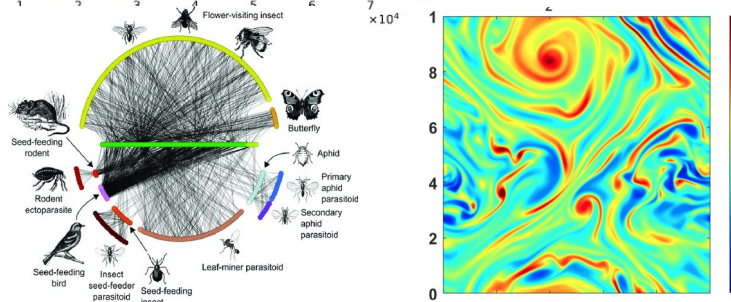
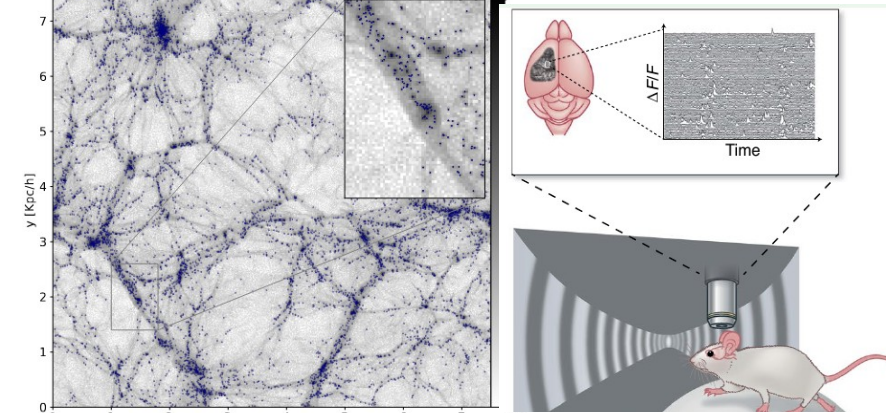
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Maximum Entropy modeling

Multiple constraints $\langle O_k(\mathbf{x}) \rangle$ with $k = 1, 2, \dots, K$

$$p_{\theta}(\mathbf{x}) \propto e^{[\mu_1 O_1(\mathbf{x}) + \dots + \mu_K O_K(\mathbf{x})]}$$



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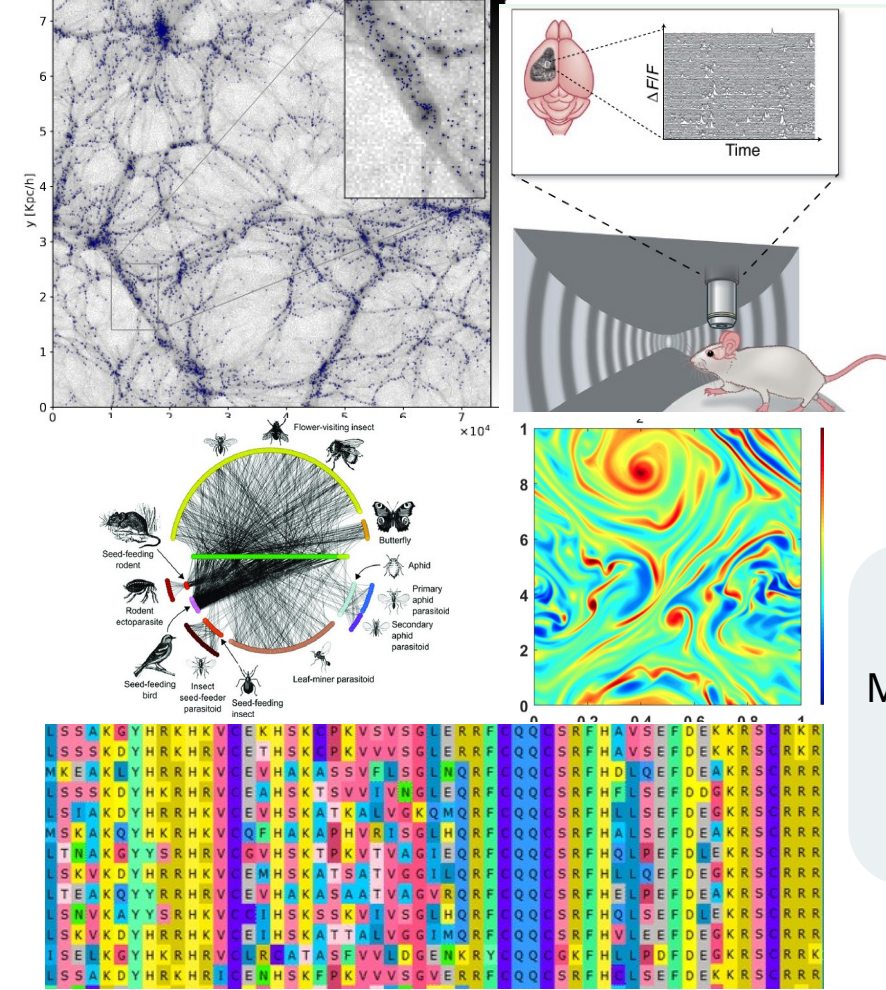
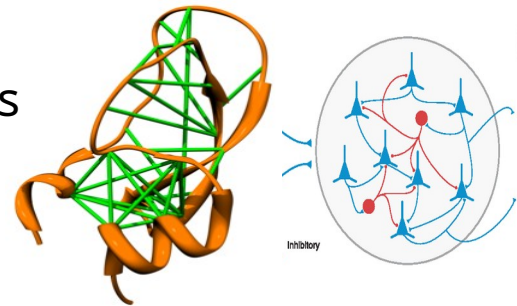
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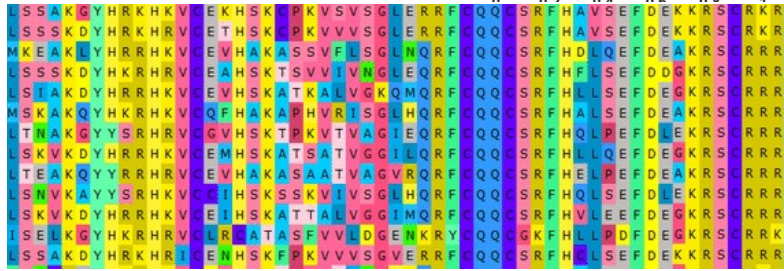
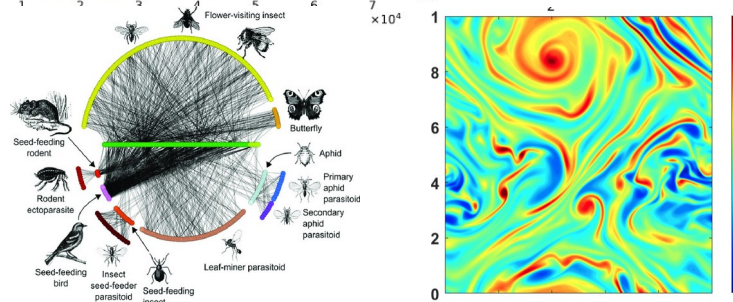
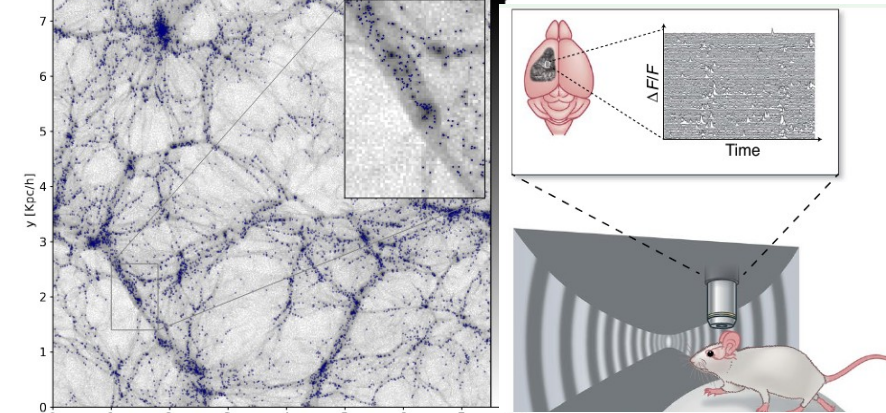
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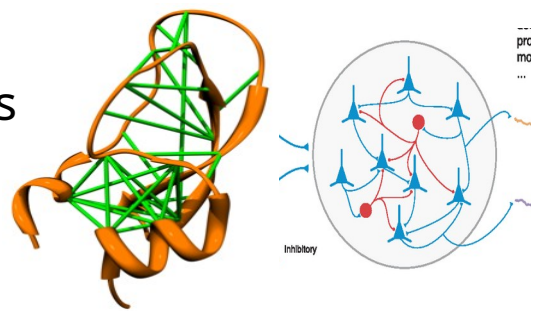
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- Advantages:**
- Simple models → Very interpretable
 - Few parameters → Reliable scarce data
- Disadvantages:**
- Too simple models → Limited expressivity

Infer effective interaction networks

$\langle \sigma_i \rangle \langle \sigma_i \sigma_j \rangle$

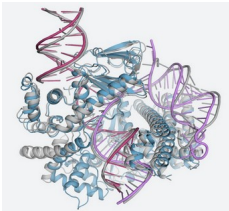


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Alternative : Generative models

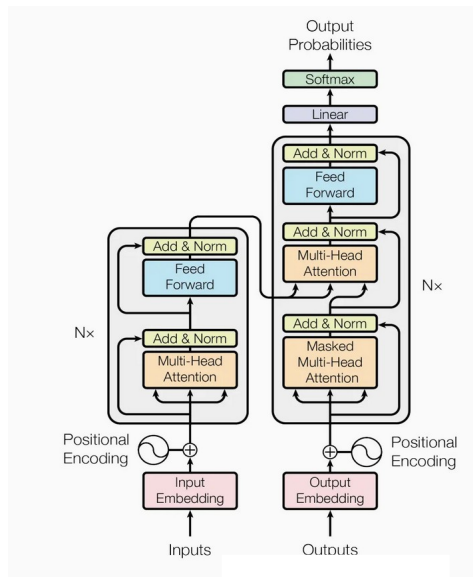
Deep Learning

Computer Science: Generative models



Advantages:
Very expressive

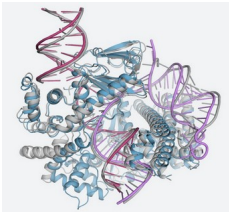
Disadvantages:
Unsustainable
Data-hungry
Black-boxes



Alternative : Generative models

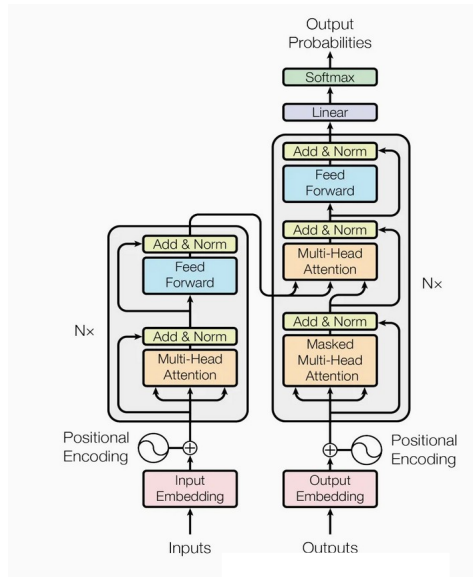
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Advantages:
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Energy-based models (EBMs)

$$p_{\text{data}} \sim p_{\theta}(\sigma) = \frac{e^{-\mathcal{H}_{\theta}(\sigma)}}{Z_{\theta}}$$



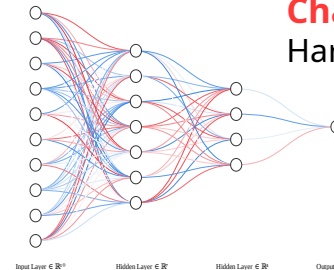
Advantages:

Highly expressive → Model complex systems
Energy & data efficient → meet scientific needs
Interpretable → Learn from data

Challenge:

Hard to train and sample from

$$\mathcal{H}_{\theta}(\sigma)$$

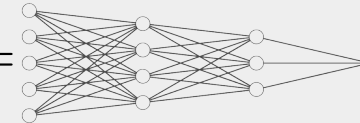




Ill. Niklas Elmehed © Nobel Prize Outreach
John J. Hopfield
 Prize share: 1/2

Ill. Niklas Elmehed © Nobel Prize Outreach
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Energy Based Models (EBMs)

$$p_{\text{data}} \sim p_{\theta}(\sigma) = \frac{e^{-\mathcal{H}_{\theta}(\sigma)}}{Z_{\theta}} \quad \mathcal{H}_{\theta}(x) =$$


Main challenge: They are very hard to train, evaluate, and sample

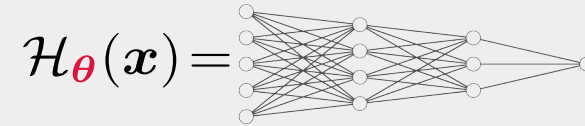


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~~Main challenge:~~ They are very hard to train, evaluate, and sample No longer true



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$$p_{\text{data}} \sim p_{\theta}(\sigma) = \frac{e^{-\mathcal{H}_{\theta}(\sigma)}}{Z_{\theta}} \quad \mathcal{H}_{\theta}(x) = \text{[Neural Network Diagram]}$$

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1) Diagnosis
 Uncontrolled Monte Carlo



- Decelle, Furtlehner, S, **NeurIPS** (2021)
- Agoritsas, Catania, Decelle, S, **ICML** (2023)



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1) Diagnosis
 Uncontrolled Monte Carlo



2) Physical origin
 Metastability
 Cascade of Phase Transitions

- Decelle, Furtlehner, S, **NeurIPS** (2021)
- Agoritsas, Catania, Decelle, S, **ICML** (2023)

- Béreux, Decelle, Furtlehner, S, **SciPost Phys.** (2023)
- Bachtis, Biroli, Decelle, S **NeurIPS** (2024)



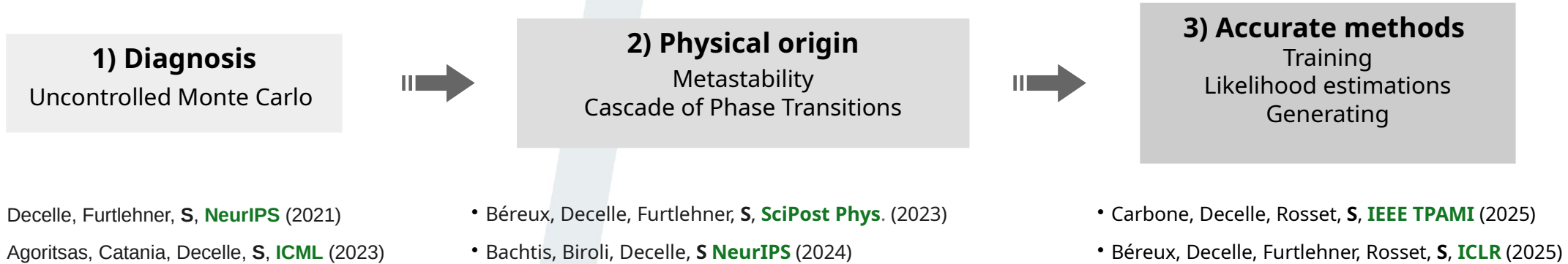
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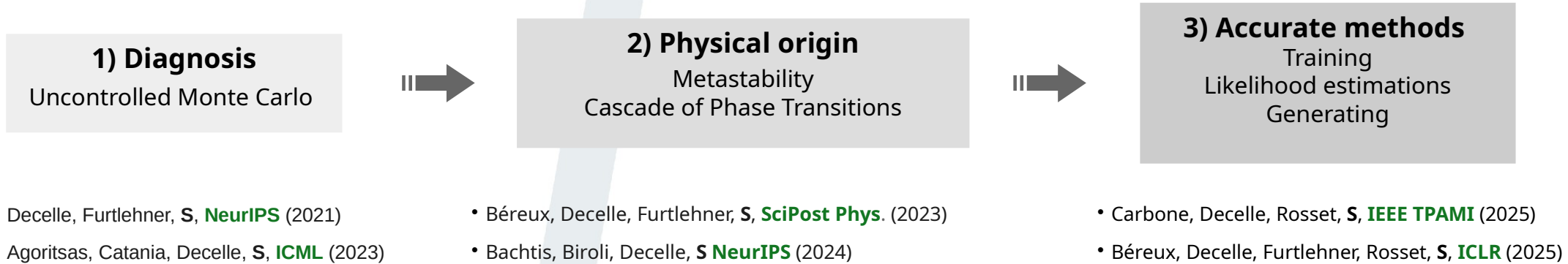
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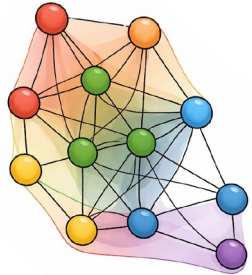
It's time to bring **EBMs** back !

Why **EBMs** ?

$$p_{\theta}(\sigma) = \frac{e^{-\mathcal{H}_{\theta}(\sigma)}}{Z_{\theta}}$$

Why **EBM_Δ** ?

Energy function


$$\mathcal{H}_{\theta}(\mathbf{S}) = - \sum_i h_i(\theta) S_i - \sum_{i < j} J_{ij}^{(2)}(\theta) S_i S_j - \sum_{i < j < k} J_{ijk}^{(3)}(\theta) S_i S_j S_k - \dots$$

←

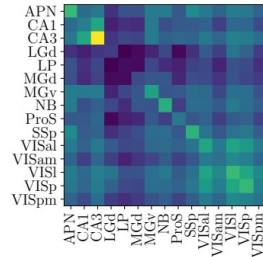
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Ising - Decelle, Furtlehner, Navas Gómez, *S*, *SciPost Phys.* (2024)

Potts - Decelle, Navas-Gómez, *S*, *accepted in Physical Review Letters* (2025)



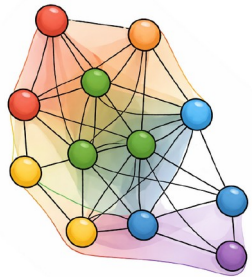
Multi-body
interaction
inference



Neural Activity - Béreux, Catania, Decelle, Mignacco, Navas Gómez, *S*. ArXiv (2026)

Why **EBM**?

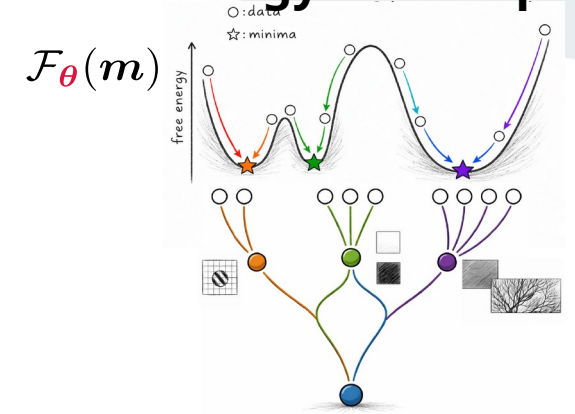
Energy function



$$\mathcal{H}_\theta(\mathbf{S}) = - \sum_i h_i(\theta) S_i - \sum_{i < j} J_{ij}^{(2)}(\theta) S_i S_j - \sum_{i < j < k} J_{ijk}^{(3)}(\theta) S_i S_j S_k - \dots$$

$$p_\theta(\sigma) = \frac{e^{-\mathcal{H}_\theta(\sigma)}}{Z_\theta}$$

Free-energy landscape

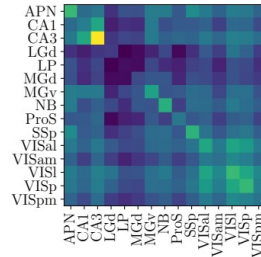


Ising - Decelle, Furtlehner, Navas Gómez, S, *SciPost Phys.* (2024)

Potts - Decelle, Navas-Gómez, S, *accepted in Physical Review Letters* (2025)



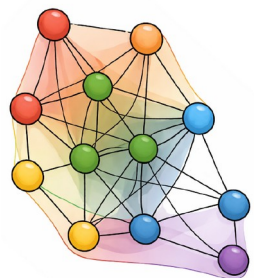
Multi-body
interaction
inference



Neural Activity - Béreux, Catania, Decelle, Mignacco, Navas Gómez, S. ArXiv (2026)

Why EBM_s?

Energy function



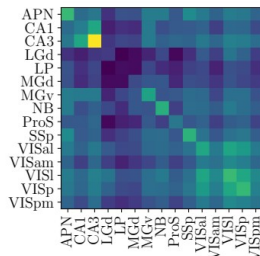
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Multi-body interaction inference



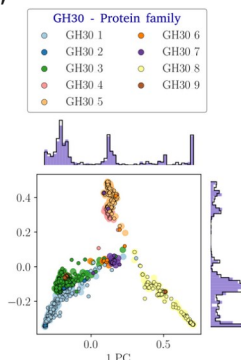
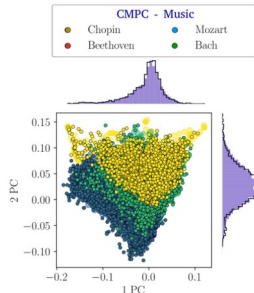
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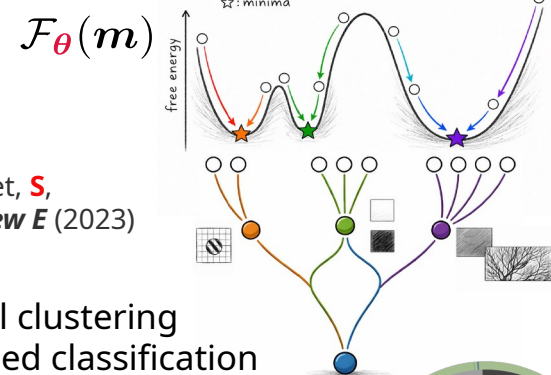
$$p_{\theta}(y) \leftarrow p_{\theta}(x|y)$$

Conditional generation

Carbone, Decelle, Rosset, S, *IEEE TPAMI* (2025)

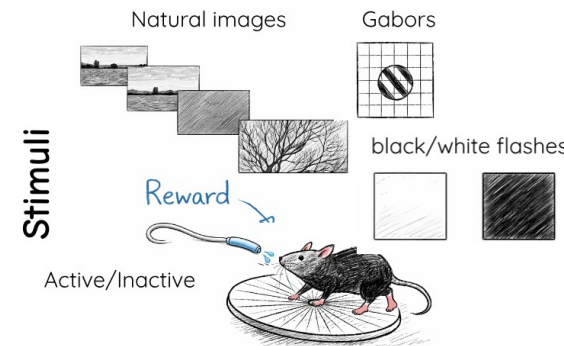
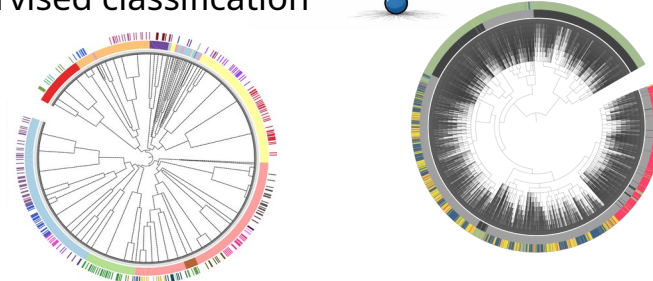


Free-energy landscape



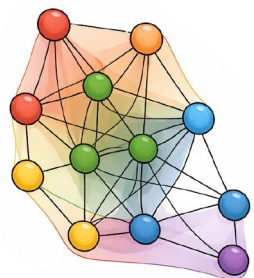
Decelle, Rosset, S, *Physical Review E* (2023)

Hierarchical clustering
Unsupervised classification



Why EBM_s?

Energy function



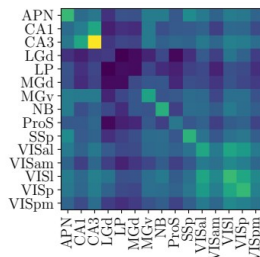
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Multi-body interaction inference



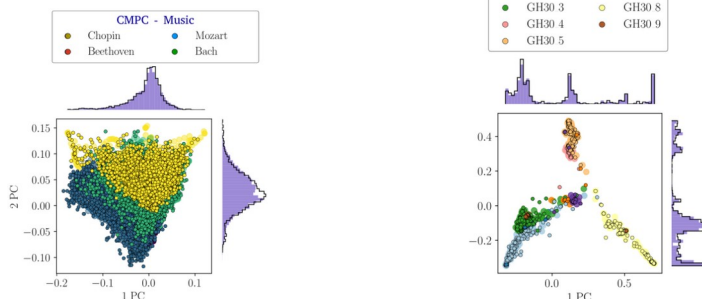
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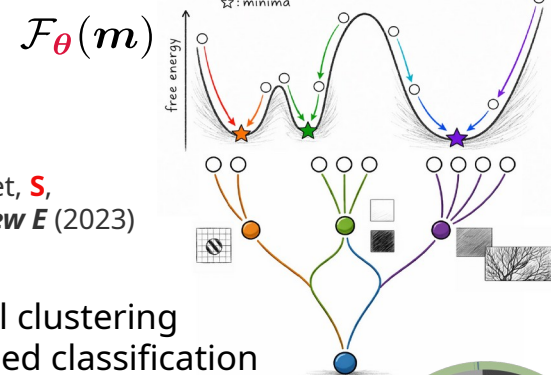
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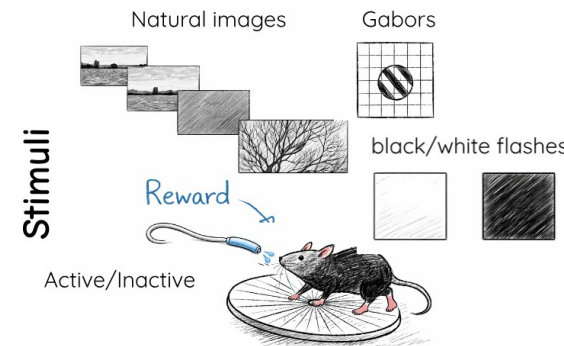
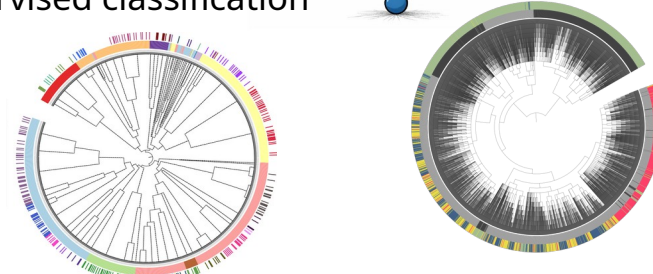


Free-energy landscape



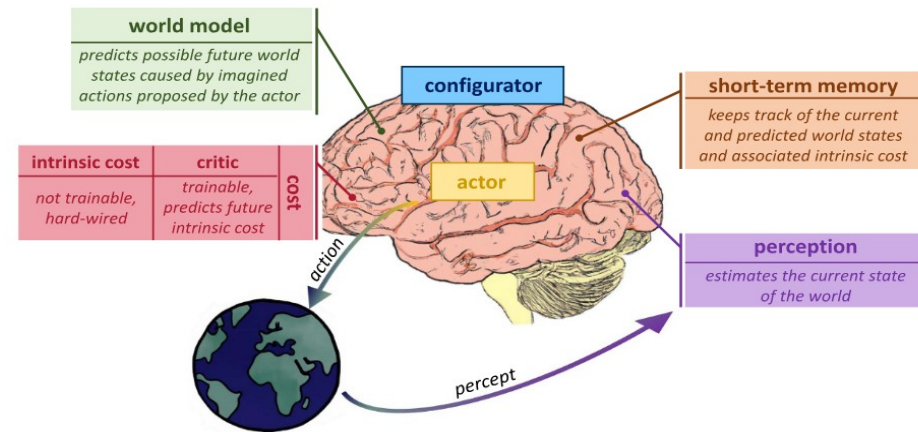
Decelle, Rosset, S, *Physical Review E* (2023)

Hierarchical clustering
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Universal toolbox for data-driven studies across fields

Why EBM_s?

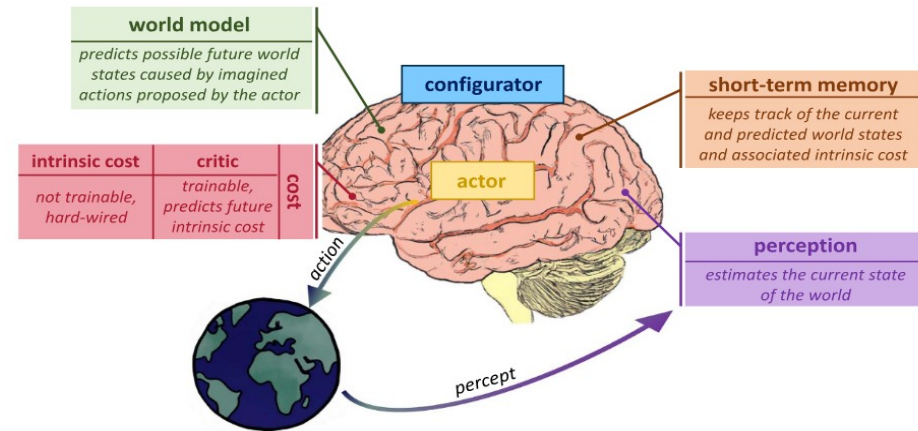
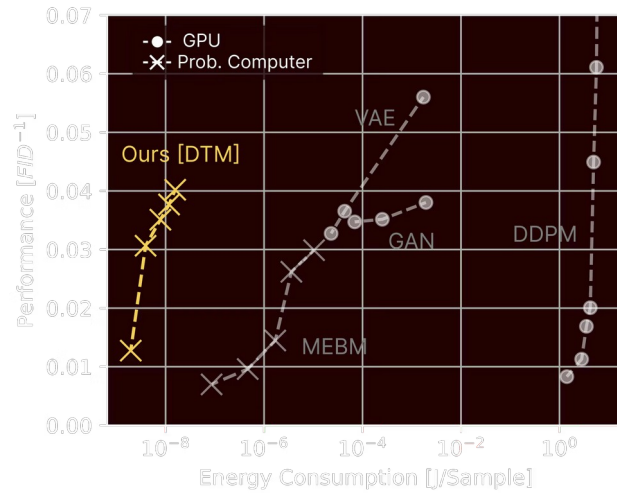


LeCun, Y. (2022). Open Review, 62(1), 1-62.

Dawid, A., & LeCun, Y. (2024). Journal of Statistical Mechanics: Theory and Experiment, 2024(10), 104011.

Why **EBMs**?

Thermodynamic sampling units (TSUs)



LeCun, Y. (2022). Open Review, 62(1), 1-62.

Dawid, A., & LeCun, Y. (2024). Journal of Statistical Mechanics: Theory and Experiment, 2024(10), 104011.

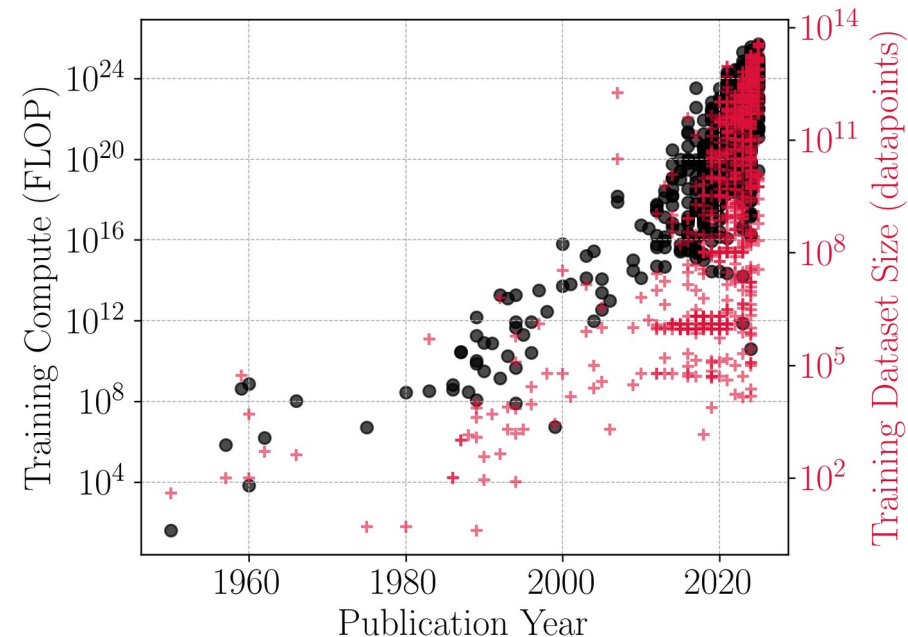
ML Challenges

- 1) Making neural networks **interpretable** and **transparent**
- 2) Challenge the prevailing **"bigger is better"** paradigm
- 3) Ensure reliability even with **limited data**



ML Challenges

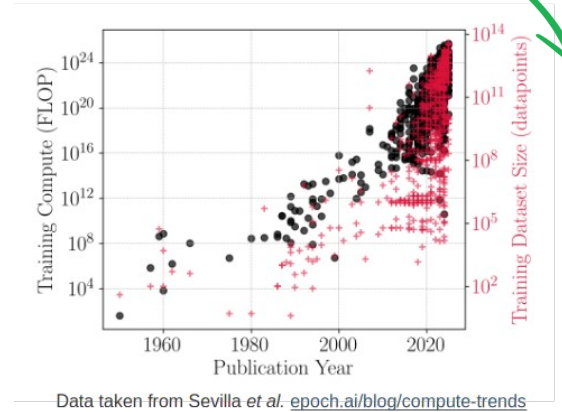
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Data taken from Sevilla *et al.* epoch.ai/blog/compute-trends

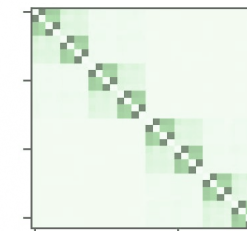
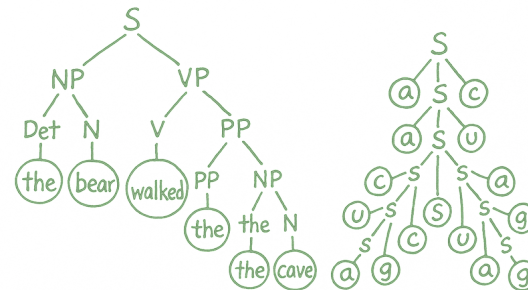
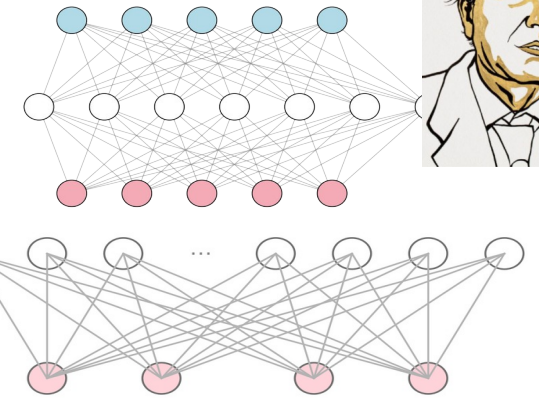
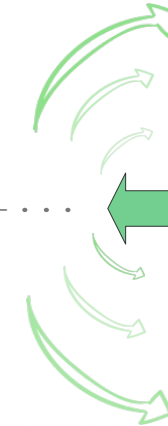
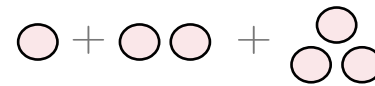
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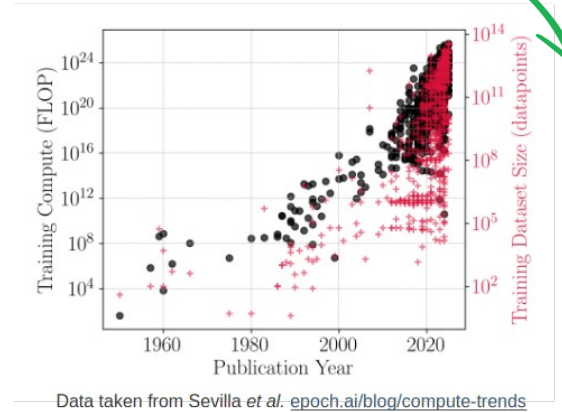
Theoretical insights

Architecture
Hyperparameter
Sampling



ML Challenges

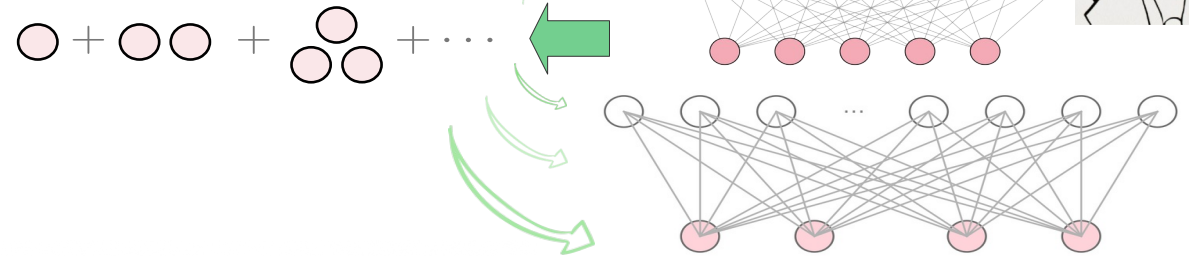
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Theoretical insights

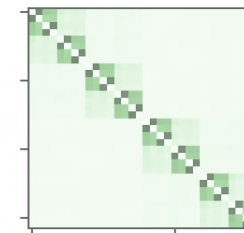
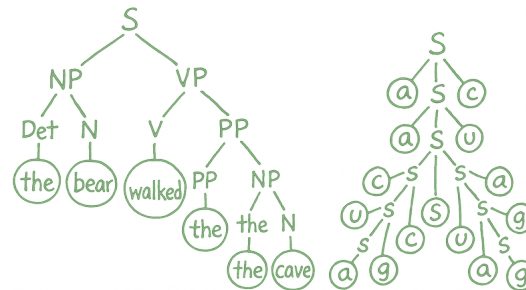
Data cleaning
 Regularization
 Early-stopping protocols
 Federated learning protocols

Architecture
 Hyperparameter
 Sampling



A Theoretical Framework For Overfitting In Energy-based Modeling

Giovanni Catania¹ Aurélien Decelle^{1,2} Cyril Furtlehner³ Beatriz Seoane¹

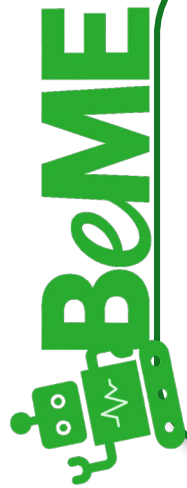




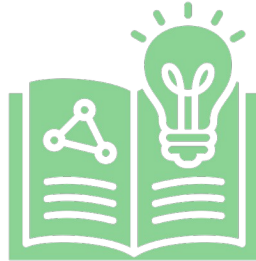
IPARCOS



UNIVERSIDAD
COMPLUTENSE
MADRID

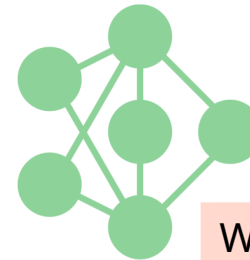


Theoretical
insights



WP4,6

Algorithms



WP2,3

Proof-of-
concept



WP1



outcome

Ready-to-use,
Fast & low-cost **code**

WP5



IPARCOS

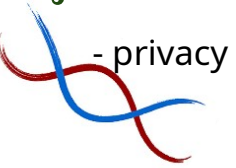


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COMPLUTENSE
MADRID

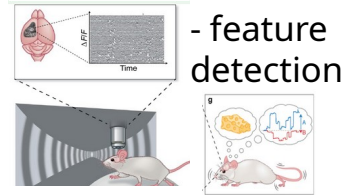
Proteins



Human
genome



Neuroscience



Turbulence



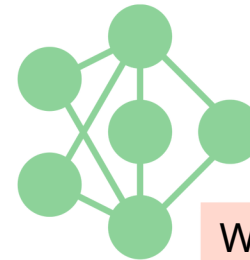
BEME

Theoretical
insights



WP4,6

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WP2,3

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IPARCOS



UNIVERSIDAD
COMPLUTENSE
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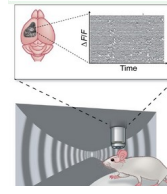
- Medical imaging
- Lattice gauge theory
- High energy experiments



Proteins



Neuroscience

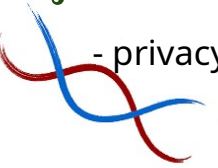


- feature detection

Turbulence



Human genome

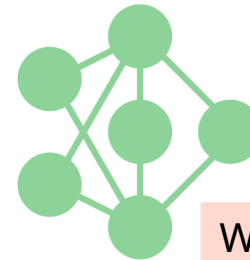


Theoretical insights



WP4,6

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