Neural network-based emulation of ISM models

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Interstellar medium and numerical simulations

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- Regression-based approximations:
  1. *k*-nearest neighbors (Smirnov-Pinchukov+2022)
  2. Random forests (Bron+2021)
  3. Neural networks (de Mijolla+2019; Holdship+2021; Grassi+2022)

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     → Less complex, so faster and allow more training data

A Meudon PDR approximation as a template

The Meudon PDR code (Le Petit+2006)

- Emulates **photo-dissociation regions** (PDRs) at equilibrium.
- This version: **4** inputs $\longmapsto \sim$ **5 000** spectral lines intensities
- Execution time $\sim$ **6 hours** and may yield **anomalies**.
- Predictions **directly comparable with observations**.

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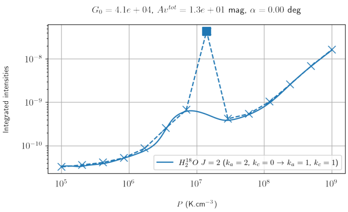

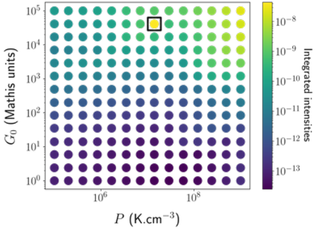

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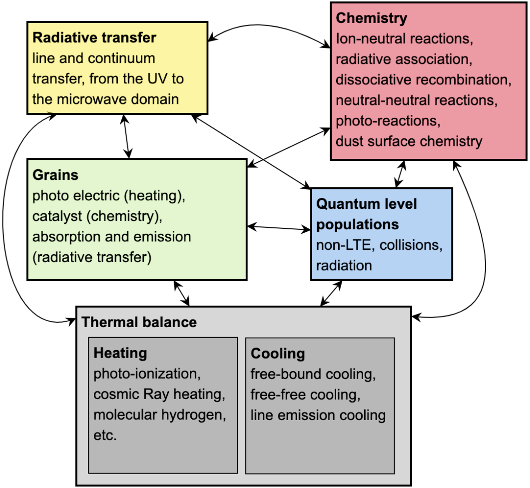

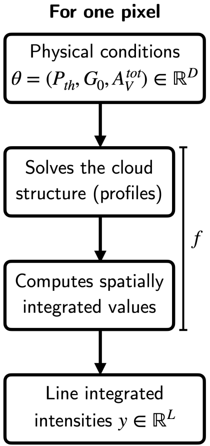

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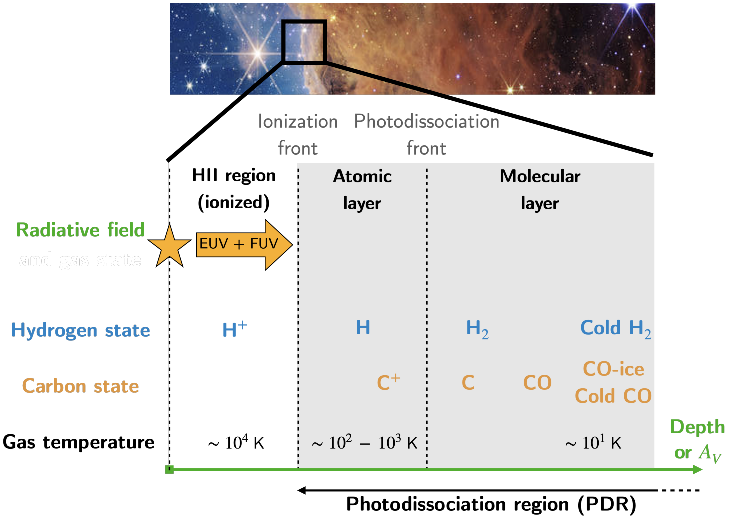

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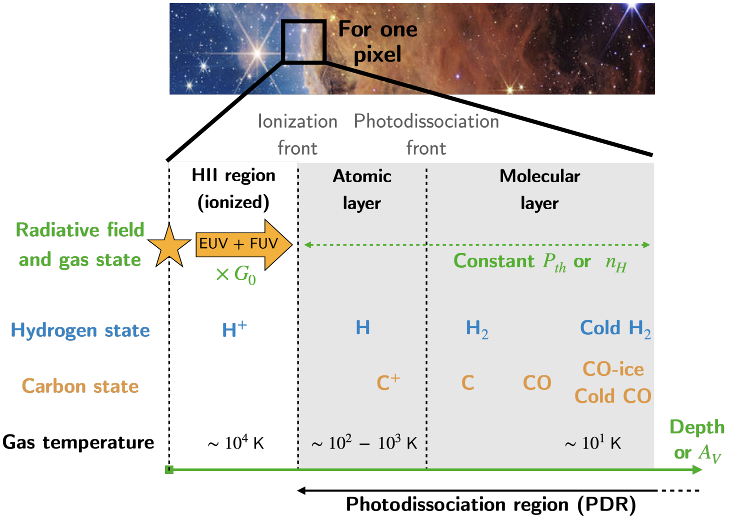

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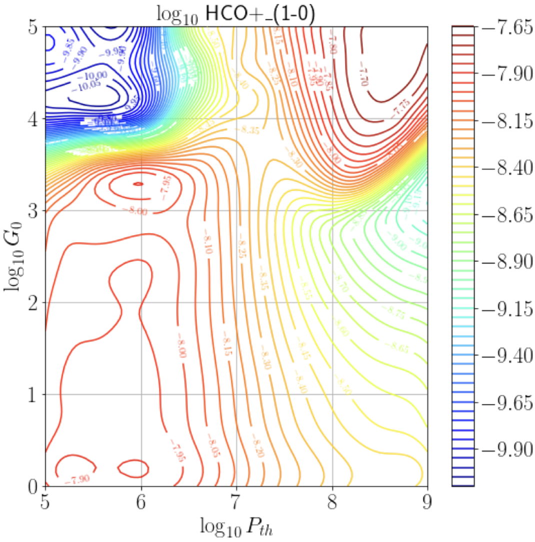
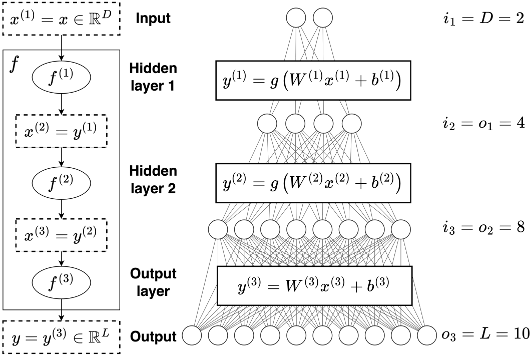


Evolutions of a standard multilayer perceptron



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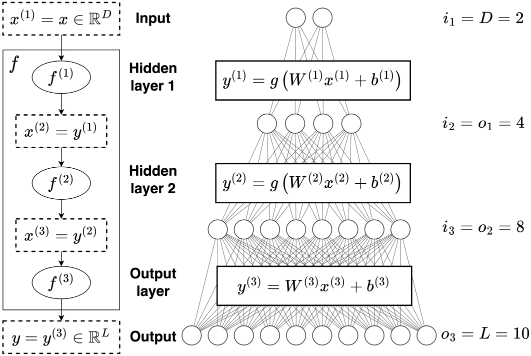

Proposition 1: polynomial expansion of inputs

Can help a network creating non-linearities. It has to be done **at execution** to ensure the network to be **fully differentiable**.

Ex: $P_2(x_1, x_2, x_3) = (x_1, x_2, x_3, x_1^2, x_1x_2, x_1x_3, x_2^2, x_2x_3, x_3^2)$

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Proposition 2: ignoring anomalies

Anomalies $\neq$ well-modeled points with sensitive behavior!

1. Training with a **robust loss** (e.g., Cauchy) to detect badly reconstructed points.
2. Use physics knowledge to determine anomalies among them.
3. New training from scratch with a **masked non-robust loss function** (e.g., MSE), **ignoring the abnormal outputs**.

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Proposition 3: outputs clustering

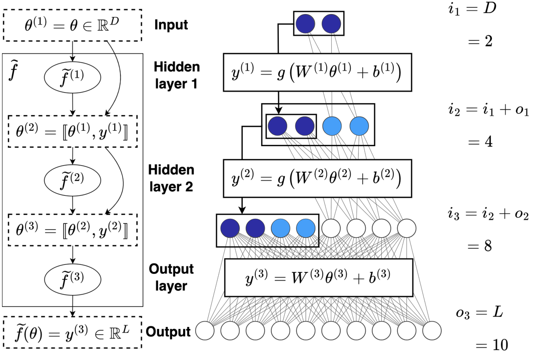
We split lines into clusters based on their **similarity**, and train **dedicated networks** for each cluster.

Method: Spectral clustering.

Evolutions of a standard multilayer perceptron

Proposition 4: reuse intermediate computations

As some outputs can be computed from other outputs, keeping track of **intermediate results** optimizes network capacities.



Dense architecture with a growing factor of 2

Results on the Meudon PDR code

We compare the results obtained with the neural network with interpolation methods.

Metrics

- **Accuracy** – error factor, a kind of symmetrized relative error, computed on **unseen data** (testing set).
- **Memory** – size of the model (whole grid for interpolations)
- **Speed** – computed on a laptop for a batch of 1 000 entries.

To be usable in inference, emulation must satisfy some constraints on these metrics.

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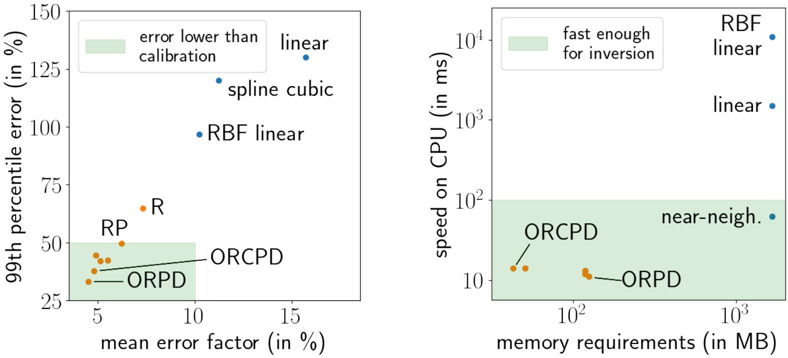

Summary of results and comparison with interpolation methods.

R: regression by an ANN **O:** outliers removal **P:** polynomial expansion

C: lines clustering **D:** dense architecture

Conclusion

Take-home messages

- Deep learning is efficient to emulate complex simulations, especially with additional constraints.
- Emulators can be plugged in Bayesian inference.
- AI benefits from physical knowledge and rigorous data analysis.

- **Paper:** Palud, Einig et al., A&A, 677, A158 (2023)
- **GitHub:** `einigl/ism-model-nn-approximation`
- **PyPI:** `pip install nnbma`

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