

Efficient deep learning approaches to denoise radioastronomy line cubes and emulate astrophysical models

L. Einig, J. Pety, P. Palud, J. Chanussot, A. Roueff, M. Gerin and the ORION-B consortium







ML-IAP/CCA-2023 contributed talk

The ORION-B dataset





- Acquired by the wide-band receiver at the IRAM-30 m
- $\blacksquare~\sim 1\,000$ h of observations
- Observations interpretation needs proper images/data processing and efficient inference procedures.

The ORION-B dataset

- \sim 30 molecular line cubes for J = 1 0 transition
- Spatially and spectrally resolved
- 1074×758 profiles
- 240 velocity channels per cube



Denoising of radio astronomy line cubes

1 Denoising of radio astronomy line cubes

2 Emulation of astrophysical codes

3 Conclusions

About denoising

Interest of denoising

- Increasing the signal-to-noise ratio is an important step to lead to discoveries.
- Necessary to find statistical relations between certain lines and physical parameters (otherwise hidden by noise).



Efficient for Earth remote sensing cubes (Licciardi+2015, Licciardi+2018).



Figure: Example of an autoencoder neural network with extrinsic and intrinsic dimensions of 10 and 3, respectively.

A locally connected AE with prior information

- Noise is pixel dependent, spectrally and spatially correlated → false signal
- Unlike Earth remote sensing cubes, very low information redundancy

 \longrightarrow need to make the best use of it



Figure: ¹³CO line and Earth image "Indian Pines" correlation matrices

Proposition 1: Loss function to help the network

- The redundancy is unsufficient for proper denoising.
- We give more information to the network with a loss function depending on a prior.
- This prior is taken from a **3D segmentation method**.

$$\mathcal{L}(\widehat{d}_{i,j}, d_{i,j}) = rac{1}{\mathcal{K}} \sum_{k=1}^{\mathcal{K}} \left\{ egin{array}{c} rac{(\widehat{d}_{i,j,k} - d_{i,j,k})^2}{\sigma_{i,j}} & ext{if probably signal + noise} \ \left| rac{\widehat{d}_{i,j,k}}{\sigma_{i,j}}
ight|^q & ext{if probably only noise} \end{array}
ight.$$

with $q \in]0,1]$ an hyperparameter than controls the sparcity.

A locally connected AE with prior information

Distant channels share almost no information

 \longrightarrow most of the weights are useless, or even counter-productive

A locally connected AE with prior information

Distant channels share almost no information

 \longrightarrow most of the weights are useless, or even counter-productive

Proposition 2: Locally connected architecture

We propose this kind of architecture where distant channels cannot be combined together.



Example of fully connected AE

Example of locally connected AE

Gaussian fitting method ROHSA

Comparison with state-of-the-art ROHSA gaussian fitting method (Marchal+2019):

- Spatially constrained Gaussian decomposition of profiles.
- Reconstruction/decomposition can perform **denoising**.



Denoising performances: residuals



Denoising performances: residuals



Lucas Einig

Emulation of astrophysical codes

1 Denoising of radio astronomy line cubes

2 Emulation of astrophysical codes

3 Conclusions

Computation time is often prohibitive for inference procedures.

Computation time is often prohibitive for inference procedures.

Usual solutions

Computation time is often prohibitive for inference procedures.

Usual solutions

Interpolation methods:

- 1 Nearest point in grid (Sheffer+2011; Sheffer+2013; Joblin+2018)
- 2 SciPy interpolation (Wu+2018; Ramambason+2022)

Computation time is often prohibitive for inference procedures.

Usual solutions

Interpolation methods:

- 1 Nearest point in grid (Sheffer+2011; Sheffer+2013; Joblin+2018)
- 2 SciPy interpolation (Wu+2018; Ramambason+2022)
- 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)

Computation time is often prohibitive for inference procedures.

Usual solutions

Interpolation methods:

- 1 Nearest point in grid (Sheffer+2011; Sheffer+2013; Joblin+2018)
- 2 SciPy interpolation (Wu+2018; Ramambason+2022)
- 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)
 - \rightarrow Less complex, so faster and allow more training data

A Meudon PDR approximation as a template

The Meudon PDR code

- Emulates **photo-dissociation regions** (PDRs) at equilibrium.
- \blacksquare 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.

A Meudon PDR approximation as a template

The Meudon PDR code

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

Overall: representative example of ISM numerical simulations.

A Meudon PDR approximation as a template

The Meudon PDR code

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

Overall: representative example of ISM numerical simulations.



Start: A multilayer perceptron to approach the simulations.

Start: A multilayer perceptron to approach the simulations.

Proposition 1: ignoring anomalies

Anomalies \neq well-modeled points with sensitive behavior!

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

Start: A multilayer perceptron to approach the simulations.

Proposition 1: ignoring anomalies

Anomalies \neq well-modeled points with sensitive behavior!

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

Proposition 2: outputs clustering to divide and conquer

Since outputs can be grouped into clusters by their similarity, it's efficient to train **dedicated networks** side by side for each cluster.

Proposition 3: reuse intermediate computations

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



Results on the Meudon PDR code

Method			Error factor			Memory	Speed
		emou	mean	99% per.	max	(MB)	(ms)
No outlier removal	near. neighbor		×13.1	×11.3	×3e5	1650	62
	linear		15.7	×2.3	×143	1650	1.5e3
	line	linear	15.7	×2.3	×144	1650	
		cubic	11.2	×2.2	×122	1650	
	sp	quintic	19.1	×2.9	×304	1650	
	Г т	linear	10.2	96.8	×99	1650	1.1e4
	BI	cubic	10.4	×2.1	×112	1650	1.1e4
	24	quintic	10.9	×2.1	×118	1650	1.1e4
	Z	R	7.3	64.8	×81	118	12
	Ā	R+P	6.2	49.7	$\times 84$	118	13

Error factor

 \rightarrow Symmetrized relative error

$$\operatorname{err}_{\%} = 100 \cdot \max\left(\frac{\hat{y}}{y}, \frac{y}{\hat{y}}\right)$$

Speed

- \rightarrow Computation of a batch of 1 000 entries on a laptop.
- R: regression by an ANN
- P: polynomial expansion
- C: lines clustering
- D: dense architecture

Results on the Meudon PDR code

	м	athod	Error factor			Memory	Speed
	141	ettiou	mean	99% per.	max	(MB)	(ms)
removal	near. neighbor		×13.1	×11.3	×3e5	1650	62
	linear		15.7	×2.3	×143	1650	1.5e3
	spline	linear	15.7	×2.3	×144	1650	
		cubic	11.2	×2.2	×122	1650	
		quintic	19.1	×2.9	×304	1650	
lie	ſT.	linear	10.2	96.8	×99	1650	1.1e4
No out	RBI	cubic	10.4	×2.1	×112	1650	1.1e4
		quintic	10.9	×2.1	×118	1650	1.1e4
	Z	R	7.3	64.8	×81	118	12
	Æ	R+P	6.2	49.7	$\times 84$	118	13

Error factor

 \rightarrow Symmetrized relative error

$$\operatorname{err}_{\%} = 100 \cdot \max\left(\frac{\hat{y}}{y}, \frac{y}{\hat{y}}\right)$$

Speed

 \rightarrow Computation of a batch of 1 000 entries on a laptop.

R: regression by an ANN

- P: polynomial expansion
- C: lines clustering
- D: dense architecture

Results on the Meudon PDR code

	Mathad		Error factor			Memory	Speed
	r	vietnou	mean	99% per.	max	(MB)	(ms)
No outlier removal	near. neighbor		×13.1	×11.3	×3e5	1 6 5 0	62
	linear		15.7	×2.3	×143	1650	1.5e3
	spline	linear	15.7	×2.3	×144	1650	
		cubic	11.2	×2.2	×122	1650	
		quintic	19.1	×2.9	×304	1650	
	RBF	linear	10.2	96.8	×99	1650	1.1e4
		cubic	10.4	×2.1	×112	1650	1.1e4
		quintic	10.9	×2.1	×118	1650	1.1e4
	Z	R	7.3	64.8	×81	118	12
	Z	R+P	6.2	49.7	×84	118	13
set	near. neighbor		×13.1	×11.6	×3e5	1 650	62
	linear		15.9	×2.4	×143	1650	1.5e3
50	spline	linear	15.9	×2.4	×144	1650	
Ē		cubic	11.1	×2.2	×120	1650	
Irai		quintic	20.0	×2.7	×285	1650	
n	RBF	linear	10.3	97.3	×97.5	1 650	1.1e4
al		cubic	10.5	×2.0	×106	1650	1.1e4
NO.		quintic	10.9	×2.0	×114	1650	1.1e4
em	ANN	R	5.1	42.0	×32.8	118	12
Outlier r		R+P	5.5	42.3	×41	118	13
		R+P+C	4.9	44.5	×44	51	14
		R+P+D	4.5	33.1	×33.8	125	11
		R+P+C+D	4.8	37.9	×37.6	43	14

Error factor

 \rightarrow Symmetrized relative error

$$\mathrm{err}_{\%} = 100 \cdot \max\left(\frac{\hat{y}}{y}, \frac{y}{\hat{y}}\right)$$

Speed

- \rightarrow Computation of a batch of 1 000 entries on a laptop.
- R: regression by an ANN
- P: polynomial expansion
- C: lines clustering
- D: dense architecture





2 Emulation of astrophysical codes





Take-home messages

- Al benefits from rigorous data analysis and physical knowledge, for example here for denoising.
- Deep learning is efficient to emulate complex simulations, especially with additional constraints.

Take-home messages

- Al benefits from rigorous data analysis and physical knowledge, for example here for denoising.
- Deep learning is efficient to emulate complex simulations, especially with additional constraints.
- Deep learning denoising by dimension reduction: Application to the ORION-B line cubes, L. Einig, J. Pety et al, A&A, 2023.
- Neural network-based emulation of interstellar medium models, P. Palud, L. Einig et al, A&A, 2023.
- https://github.com/einigl
- $\blacksquare \ \texttt{https://pypi.org/project/nnbma} \longrightarrow \texttt{pip install nnbma}$