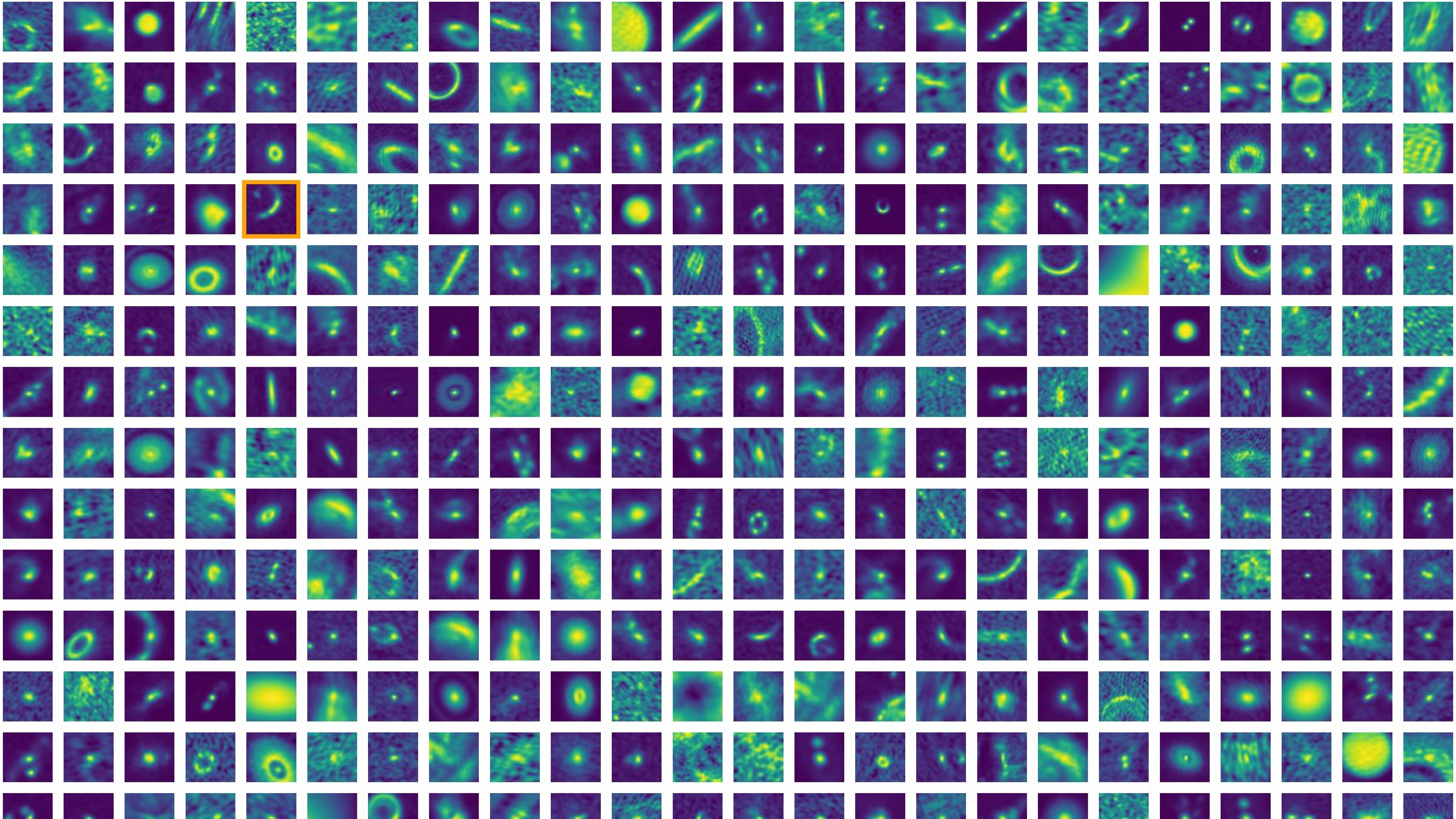
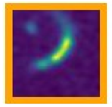
“You might also like these images”

unsupervised affine-transformation-independent representation learning for the ALMA Science Archive

Felix Stoehr, ESO/ALMA

Introduction





“show me similar images“

Introduction

Big picture: astronomy

- Data-growth in astronomy is exponential
- Astronomers ~~will be~~ are the rare resource (ADASS 2014)
- Machine learning to the rescue (ADASS 2018)

Introduction

Big picture: archives

- Daniel Durand (ADASS 2015): “The next frontier for science archives is to make the **content** of the data searchable”

- ALMA first small steps
  - Text-based similarity search using NLP
  - Previews with line-finding and line-identification (ADMIT, P. Teuben)

- Now image similarity, inspired by Josh Peek’s ADASS talk (2018)

Introduction

Big picture: fastronomy

It is not good enough that scientists can do what they need to do.
They also have to be able to do it **fast**.

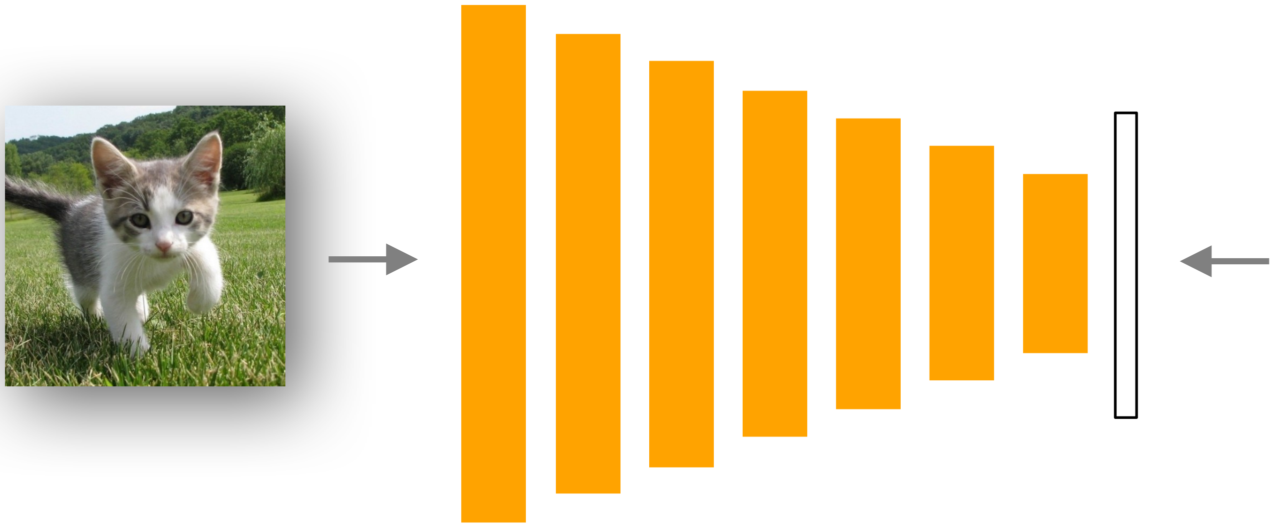
fastronomy

Let scientists concentrate on science

Supervised learning

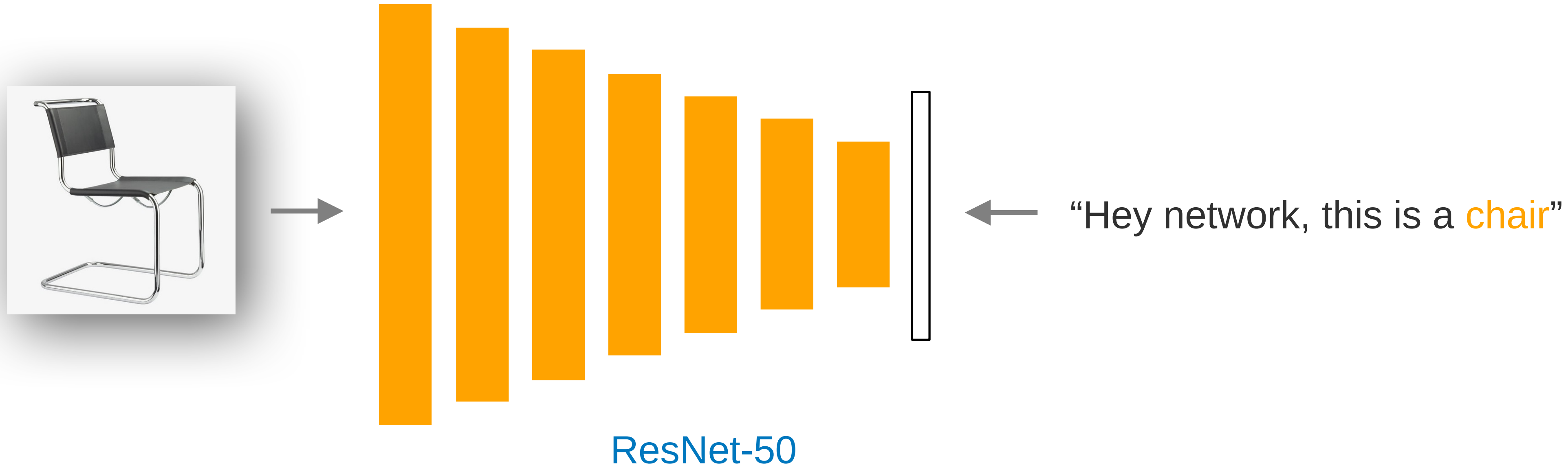
Supervised

Deep learning with labeled data



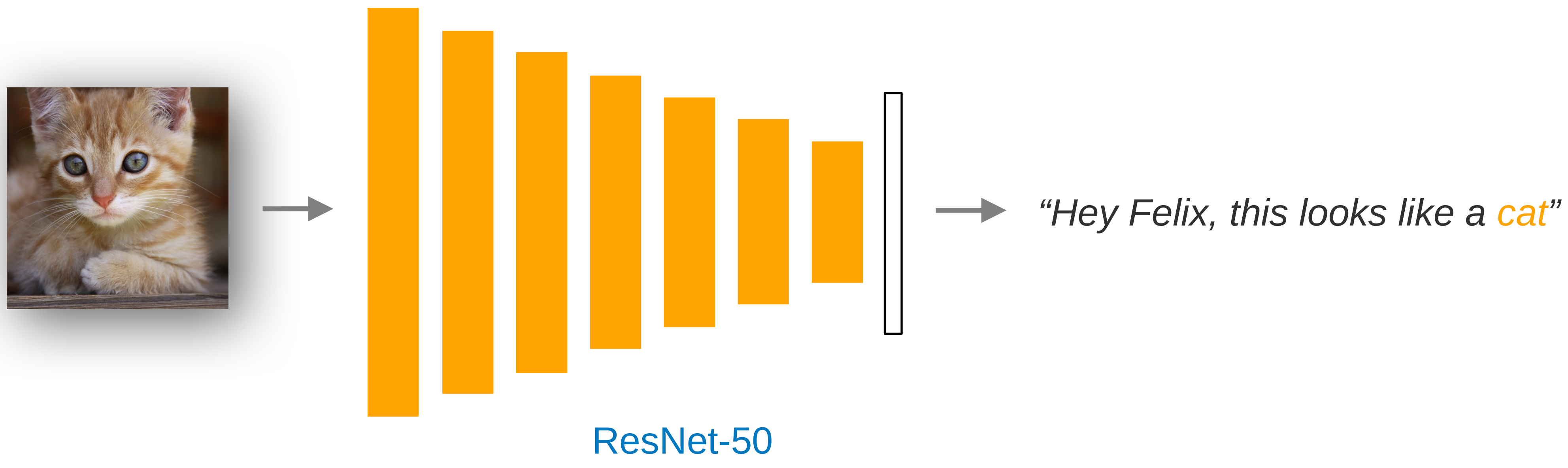
Supervised

Deep learning with labeled data



Supervised

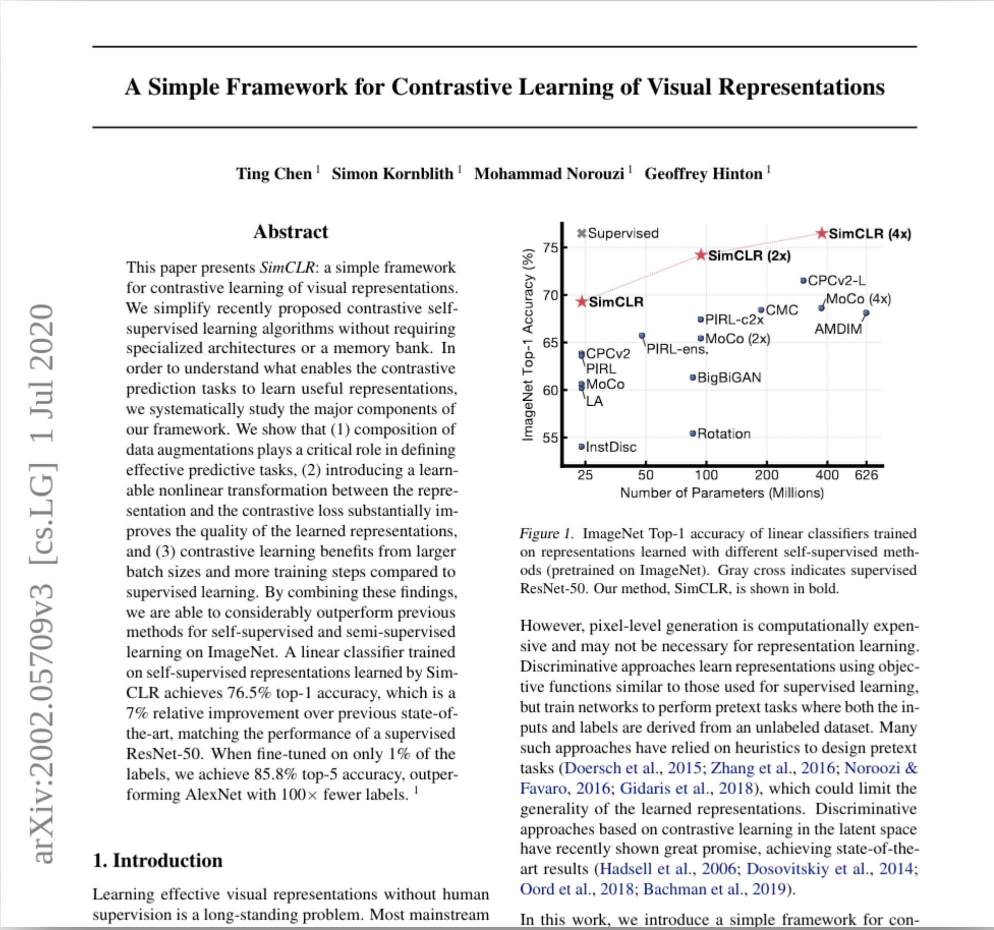
Deep learning with labeled data



Contrastive Learning

Unsupervised

SimCLR: self-supervised representation learning



arXiv:2002.05709v3 [cs.LG] 1 Jul 2020

A Simple Framework for Contrastive Learning of Visual Representations

Ting Chen [1] Simon Kornblith [1] Mohammad Norouzi [1] Geoffrey Hinton [1]

Abstract

This paper presents *SimCLR*: a simple framework for contrastive learning of visual representations. We simplify recently proposed contrastive self-supervised learning algorithms without requiring specialized architectures or a memory bank. In order to understand what enables the contrastive prediction tasks to learn useful representations, we systematically study the major components of our framework. We show that (1) composition of data augmentations plays a critical role in defining effective predictive tasks, (2) introducing a learnable nonlinear transformation between the representation and the contrastive loss substantially improves the quality of the learned representations, and (3) contrastive learning benefits from larger batch sizes and more training steps compared to supervised learning. By combining these findings, we are able to considerably outperform previous methods for self-supervised and semi-supervised learning on ImageNet. A linear classifier trained on self-supervised representations learned by SimCLR achieves 76.5% top-1 accuracy, which is a 7% relative improvement over previous state-of-the-art, matching the performance of a supervised ResNet-50. When fine-tuned on only 1% of the labels, we achieve 85.8% top-5 accuracy, outperforming AlexNet with 100× fewer labels. [1]

1. Introduction

Learning effective visual representations without human supervision is a long-standing problem. Most mainstream

Figure 1. ImageNet Top-1 accuracy of linear classifiers trained on representations learned with different self-supervised methods (pretrained on ImageNet). Gray cross indicates supervised ResNet-50. Our method, SimCLR, is shown in bold.

However, pixel-level generation is computationally expensive and may not be necessary for representation learning. Discriminative approaches learn representations using objective functions similar to those used for supervised learning, but train networks to perform pretext tasks where both the inputs and labels are derived from an unlabeled dataset. Many such approaches have relied on heuristics to design pretext tasks (Doersch et al., 2015; Zhang et al., 2016; Noroozi & Favaro, 2016; Gidaris et al., 2018), which could limit the generality of the learned representations. Discriminative approaches based on contrastive learning in the latent space have recently shown great promise, achieving state-of-the-art results (Hadsell et al., 2006; Dosovitskiy et al., 2014; Oord et al., 2018; Bachman et al., 2019).

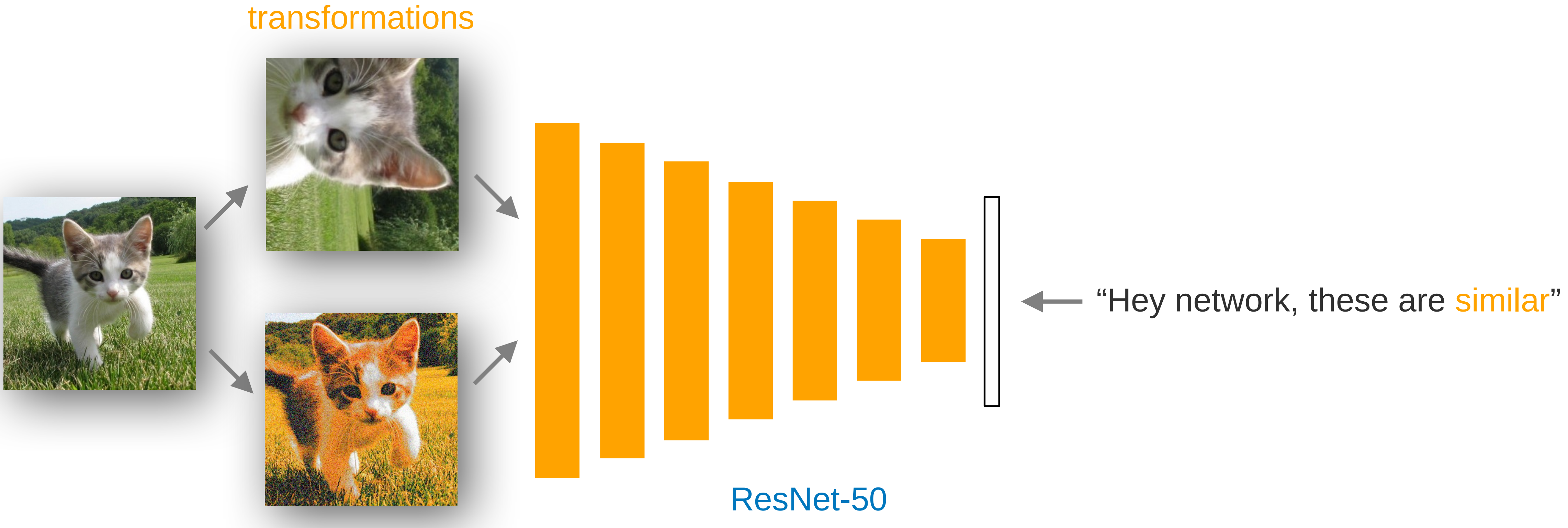
In this work, we introduce a simple framework for con-

Yann LeCun (2023)
"Self-Supervised Learning has taken over the world"

- arXiv/2002.05709
  Chen, T., et al. (2020), Google Brain Team
- library:
  https://github.com/vturrisi/solo-learn
  jmlr: Turrisi da Costa, V., et al. (2022)

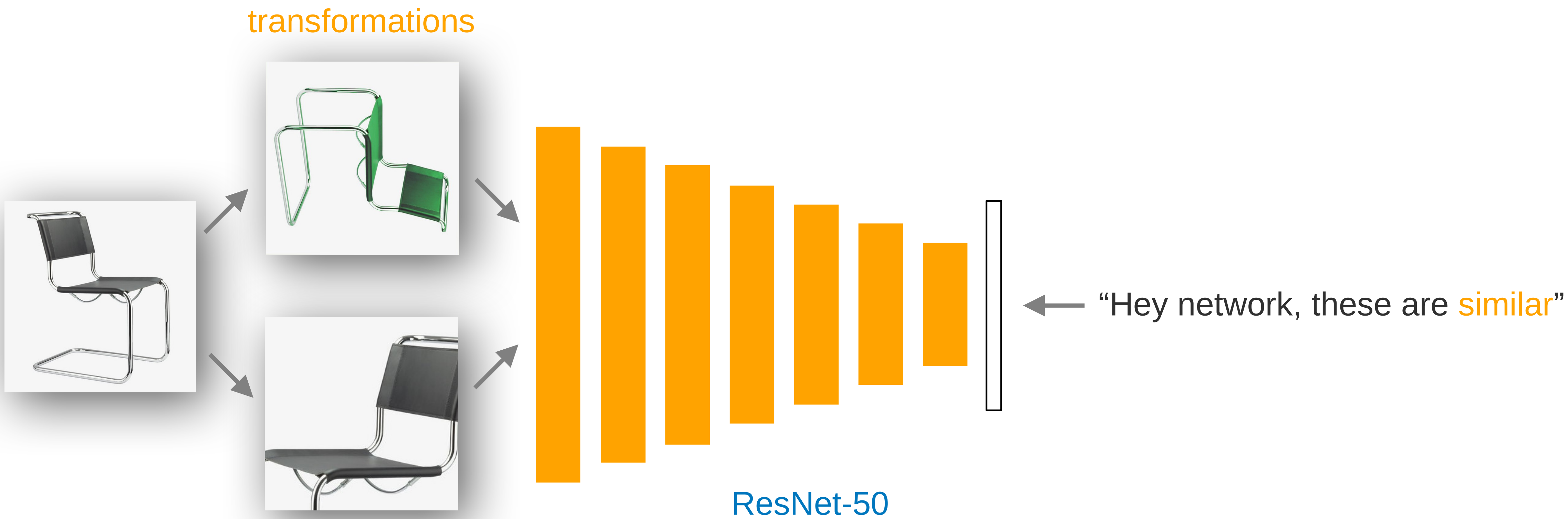
Unsupervised

SimCLR: Contrastive representation learning



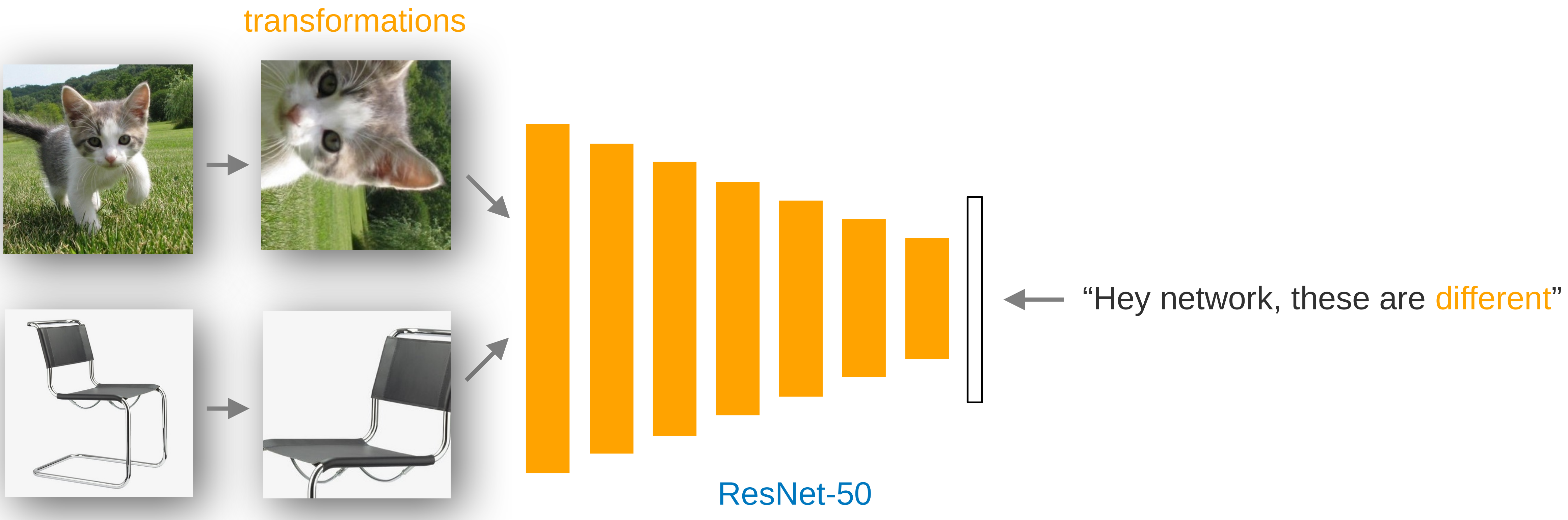
Unsupervised

SimCLR: Contrastive representation learning



Unsupervised

SimCLR: Contrastive representation learning



SimCLR

Changes needed for astronomical images

- Add affine transformations
  - rotation (arbitrary angle)
  - shear
  - scale
  - (flip, offset)
  - logscale (TBD)

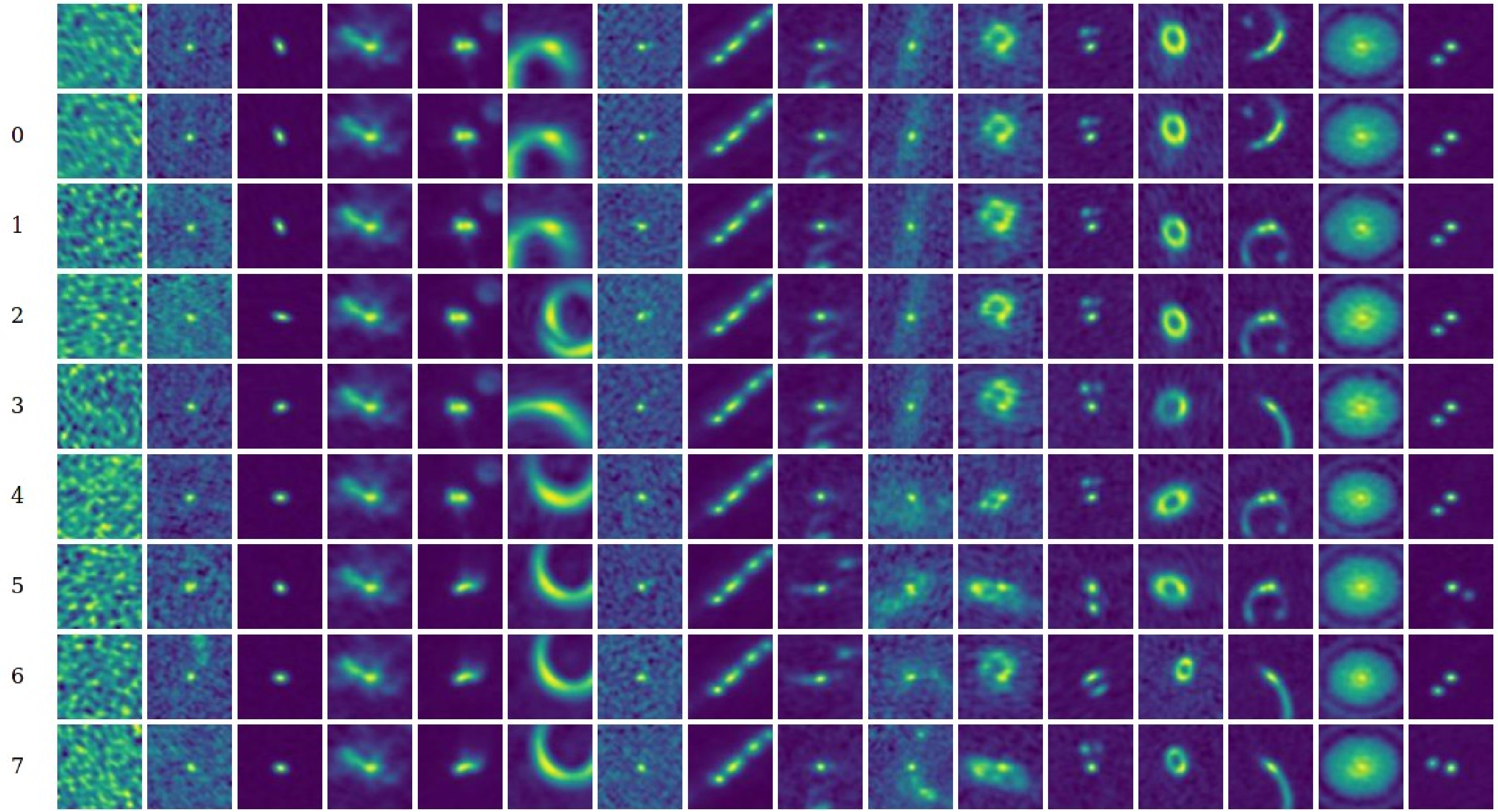
- Removal of the striping of the first ResNet layers

- Optimization: hyperparameter search (12 parameters)

Results

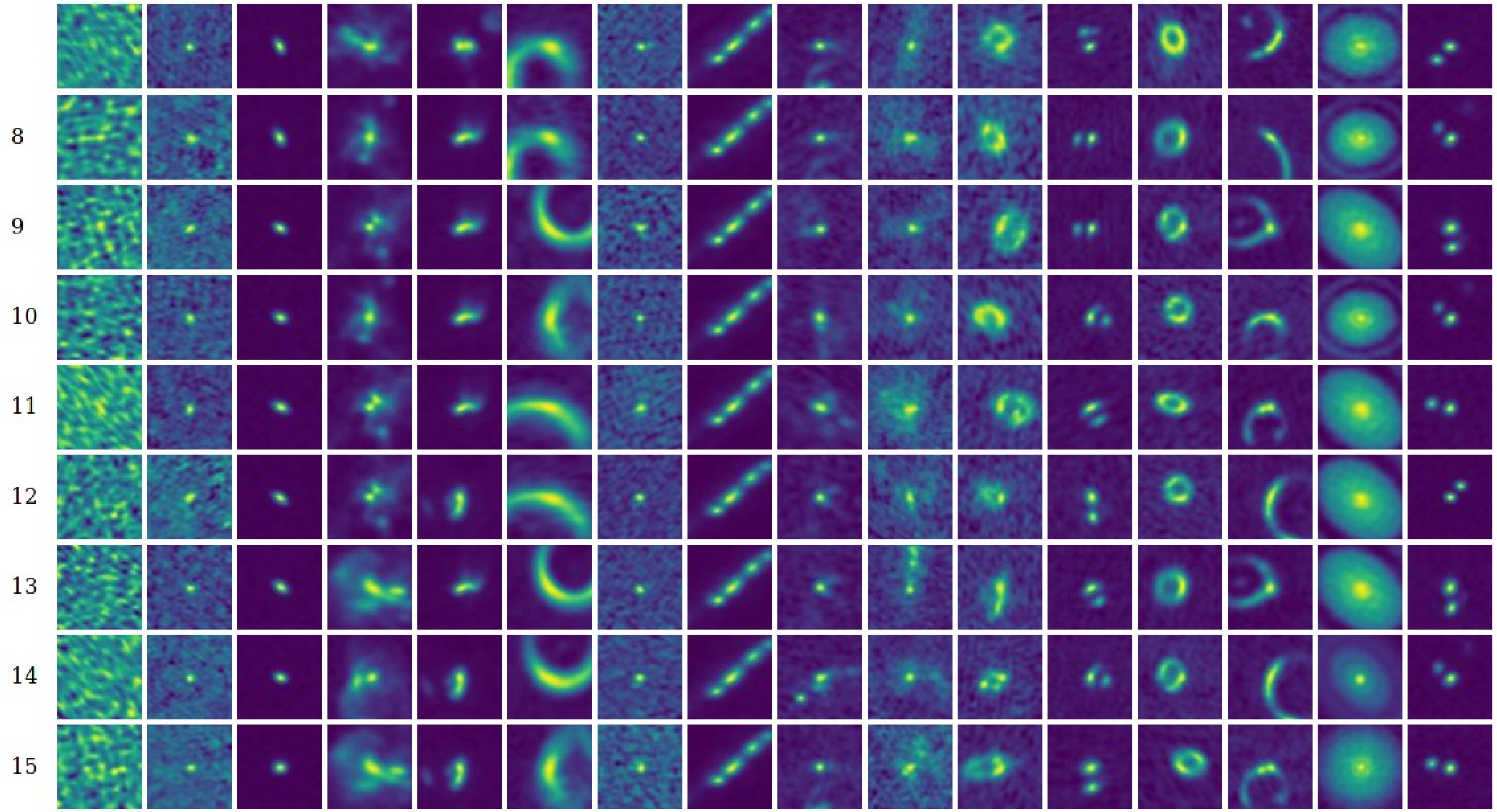
Results

ALMA image similarity



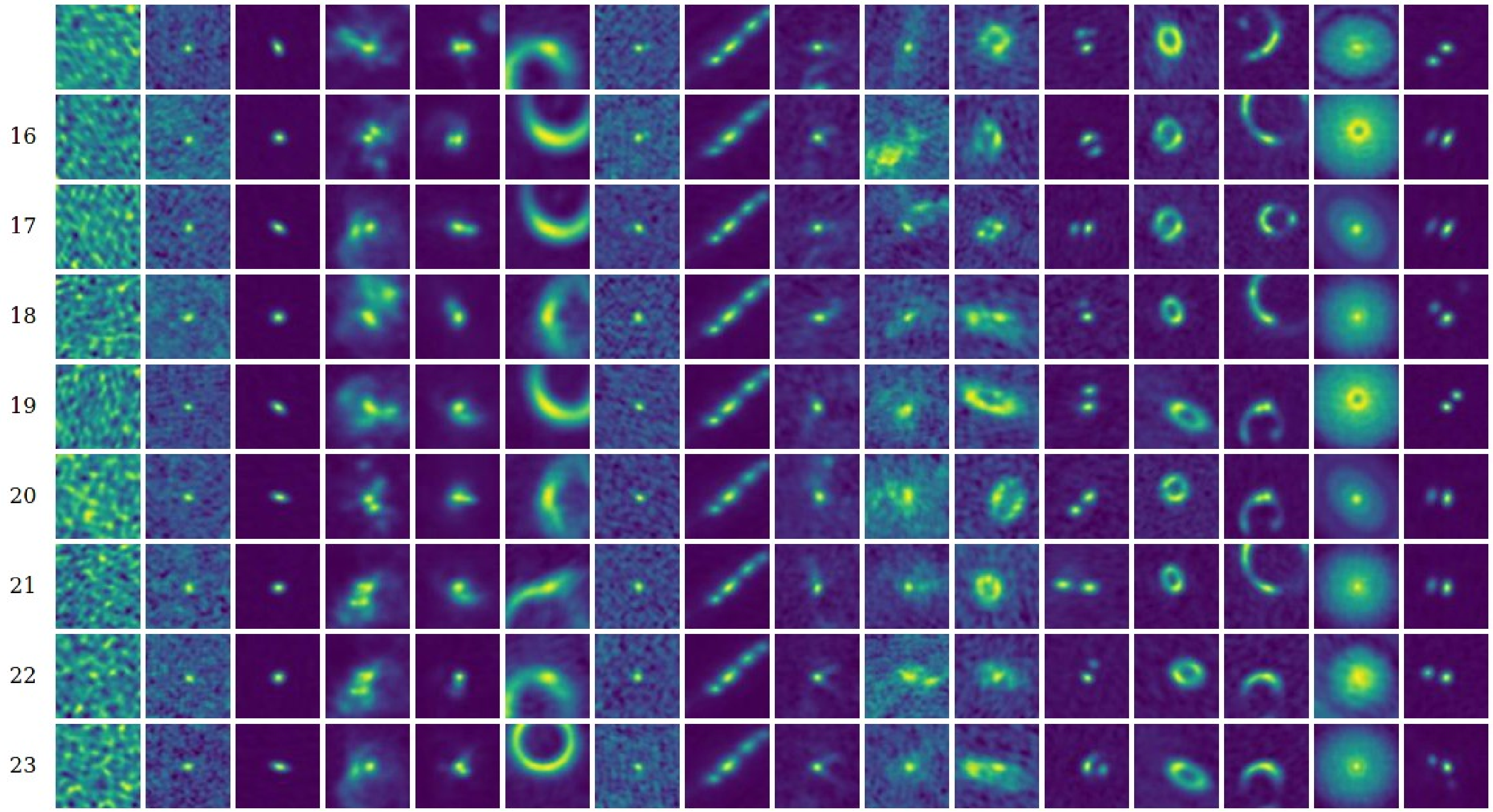
Results

ALMA image similarity



Results

ALMA image similarity



Workflow

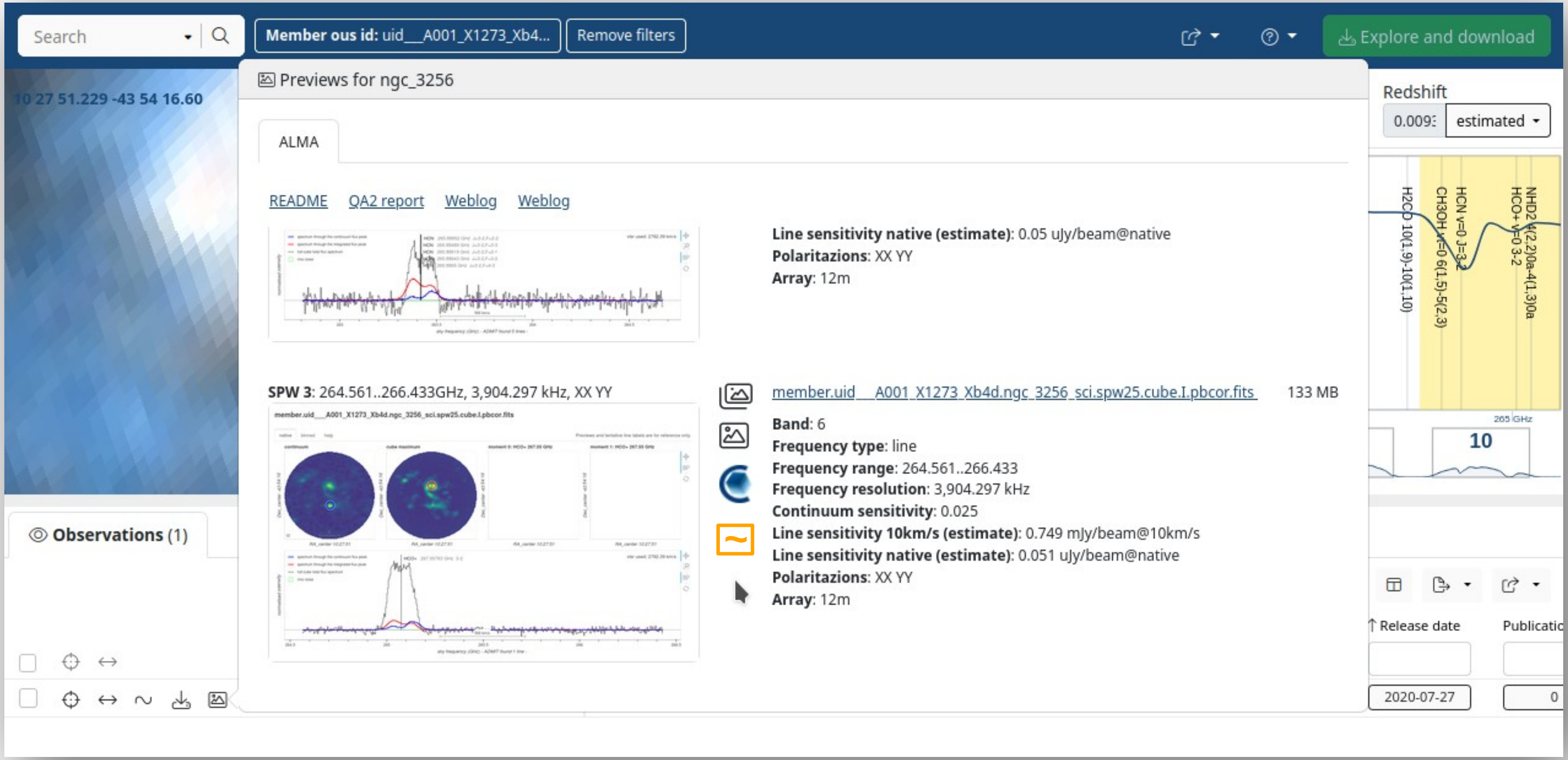
Workflow

Training, inference and similarity evaluation

- Training: need to train for many epochs (e.g. 1000) O(N)
- Inference: evaluate the model for each image [N, 2048] O(N)
- Compute the similarity of each image with all others O(N log(N))
  - Trick 1: normalize the vectors ⇒ can use L2 instead of cosine distance
  - Trick 2: use kd-tree to find the 1000 most-similar images
  - Trick 3: instead of scikit-learn (CPU) use cuml (GPU): 60x faster
- Final data file: similarity matrix [N, 1000]
- All processes ~O(N) [~16h on 3 GPUs for 1000 epochs] ⇒ fully scalable

Workflow

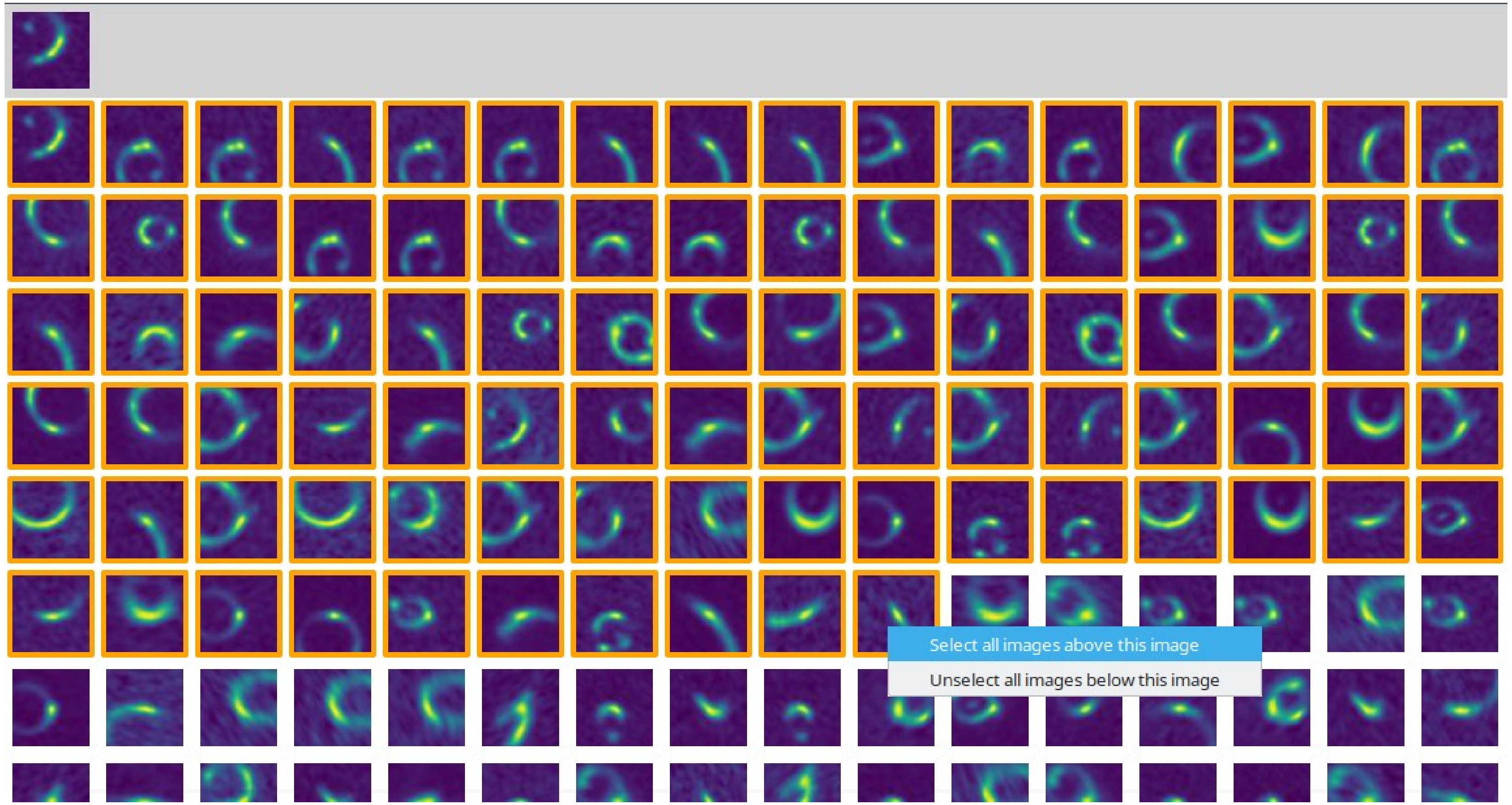
Webinterface



Prototype

Prototype

The interface



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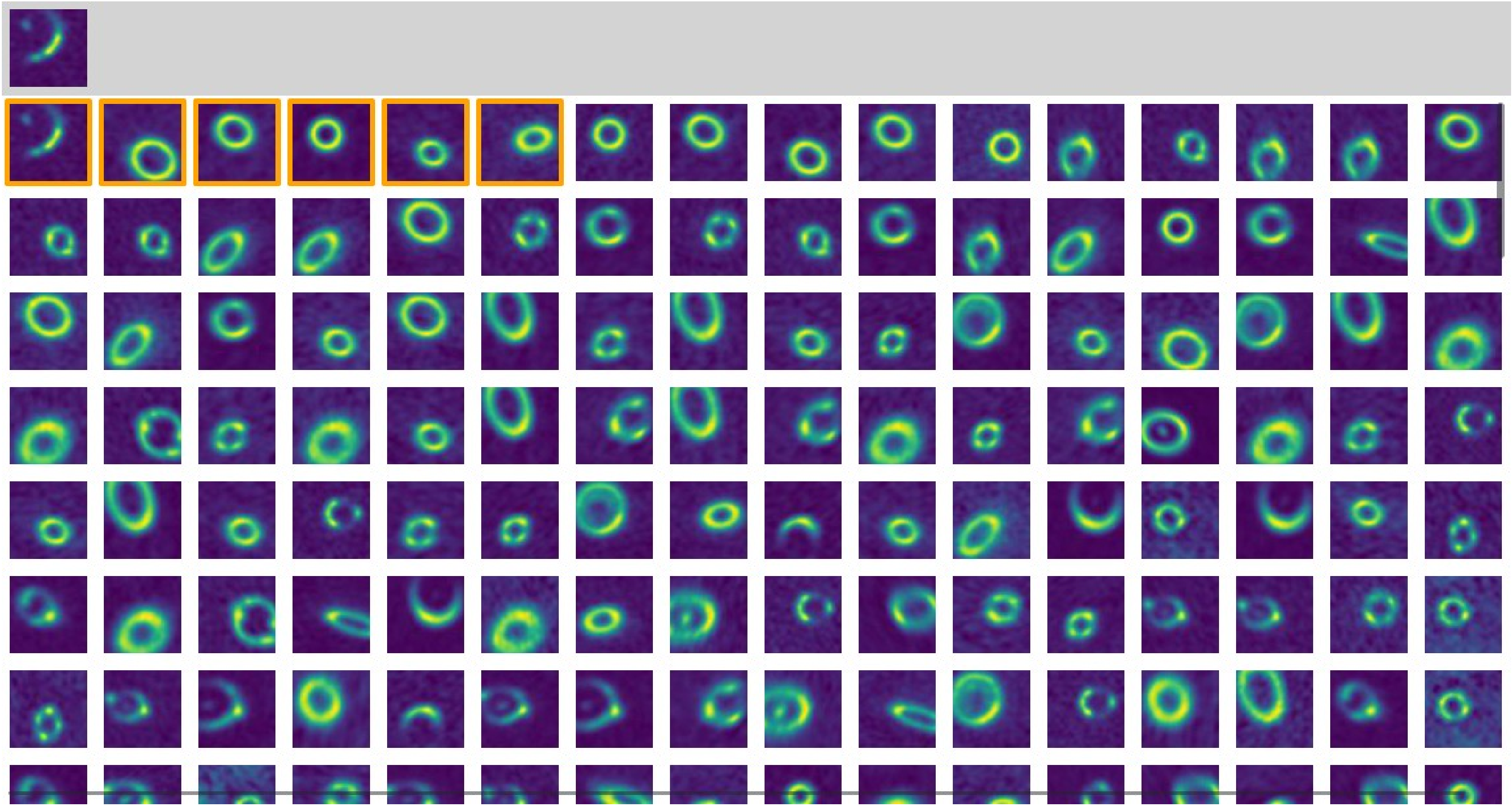

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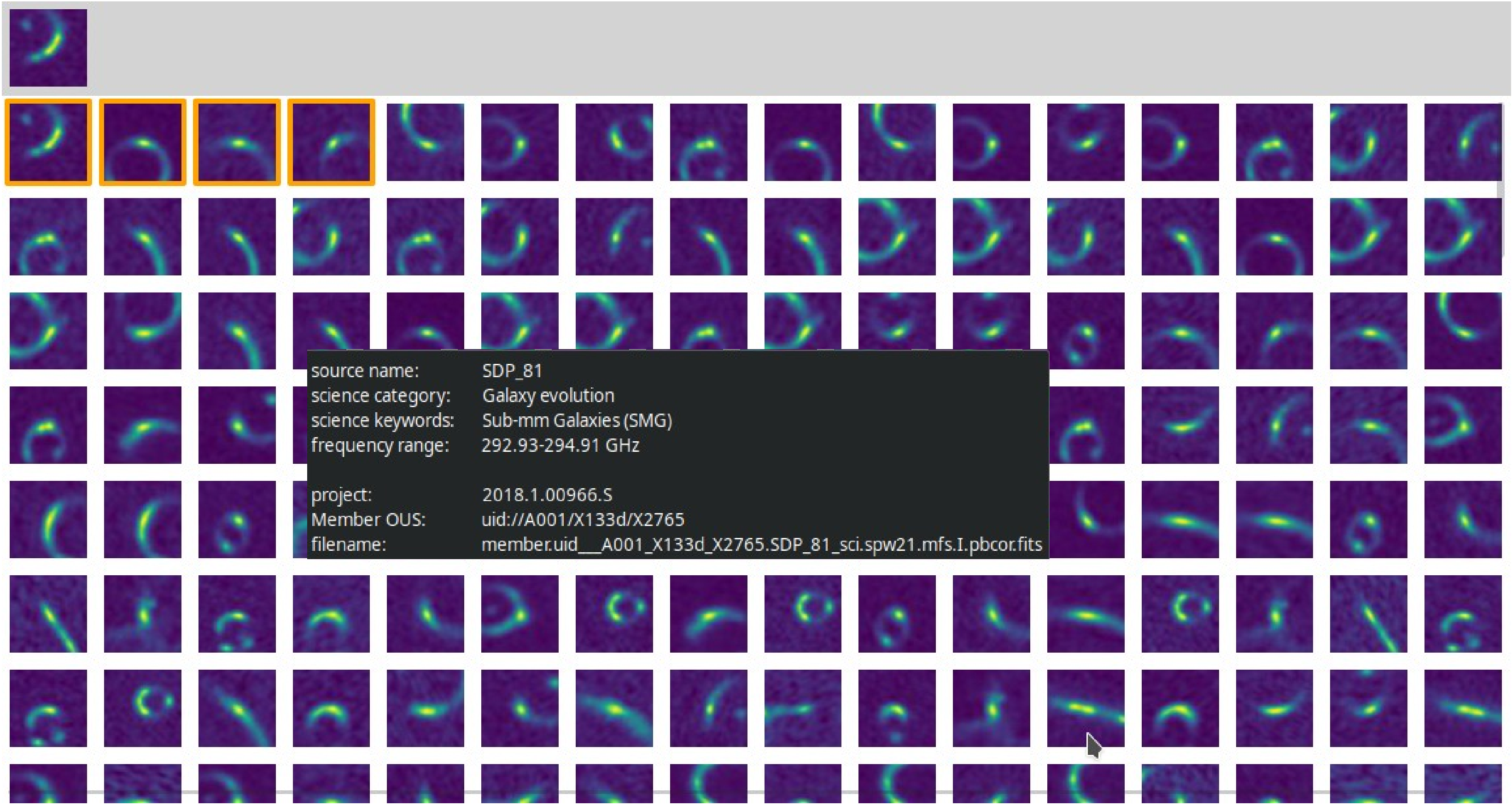

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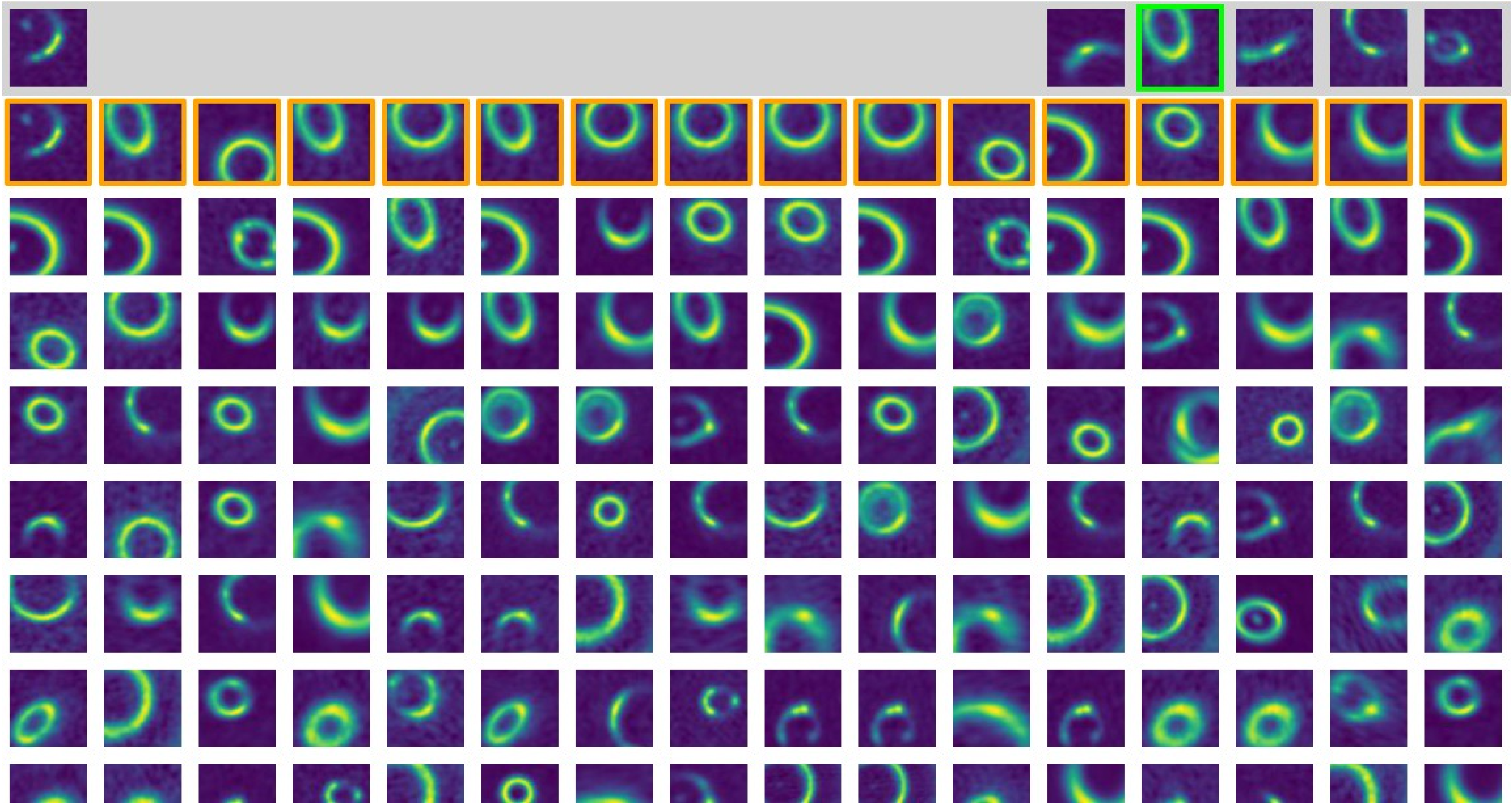

Todo

Todo

The outlook

- Scientific validation
  - Have astronomers select similar (and different) images to get a test-set
  - Use the results
    - to optimize the hyperparameters
    - directly in the training
  - In production: record all selections done on the interface and continuously improve the model

- Training per science category (or at least galactic vs. extragalactic)?

- Nice-to-have:
  - Upload image (this will require GPU access)

Conclusions

Conclusions

- Self-supervised CLR is a breakthrough for representation learning and image similarity
- An image similarity interface can be a valuable asset for Science Archives in astronomy
- Can be done for continuum and line cubes (through peak-flux image computation)
- Discovery can be sped up vastly (fastronomy)
- All similarity information can be pre-computed and the interface can make use of standard web technology without the need for GPU access
- Can provide refinement of the result through the image selections and quick select
- Can improve the model continuously with recorded selections

- Hyperparameters do have substantial influence over the result
- There is no objective ‘similarity’ for astronomical images and what astronomers need depends strongly on their science case even for the same initial image
- Finds similar images but not necessarily all similar images