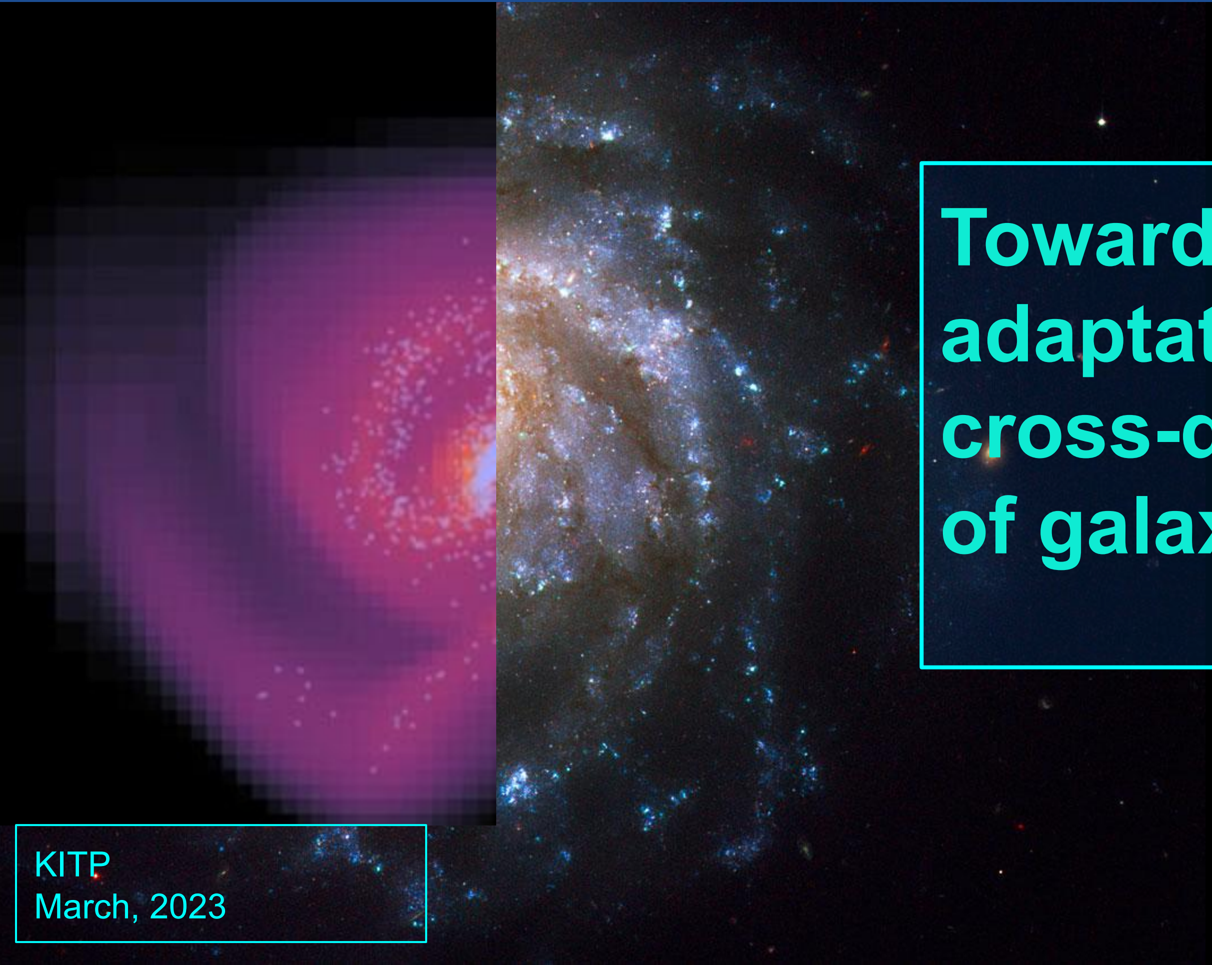
Fermilab U.S. DEPARTMENT OF ENERGY Office of Science



Towards flexible domain adaptation methods for cross-datasets studies of galaxies

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KITP
March, 2023

Vision of the Future

- **Real-time:**
  - data handling,
  - decision making
  - detection of interesting events
  - inference
- **Automated experiments**
- **Working with big data** later in the process

Rubin LSST

~ 20 TB / day
~ 100 PB total by DR11

Often research starts from simulations…
…but when AI gets involved…
…we face some challenges.

Talk Outline

1. Domain Shift Problems

2. Domain Adaptation

3. Universal Domain Adaptation

4. Future Challenges

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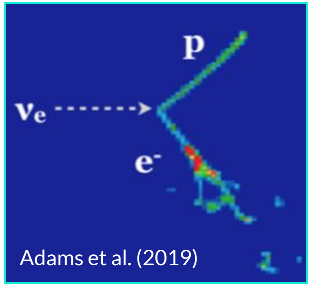
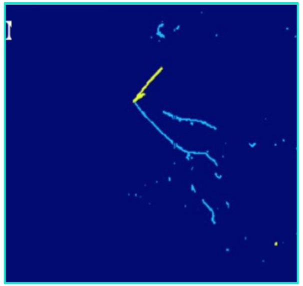
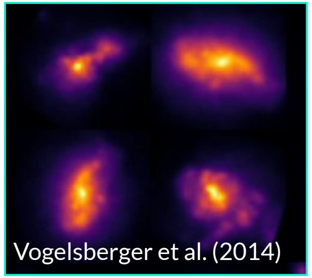
1. Domain Shift Problems
2. Domain Adaptation
3. Universal Domain Adaptation
4. Future Challenges

Combining Datasets

All areas of Fermilab science often need to create **model trained on simulated data, that also work on real detector data**!

DATASET SHIFT

	SIMULATED	REAL
MicroBooNE (neutrinos)	 Adams et al. (2019)	
Illustris / Hubble (merging galaxies)	 Vogelsberger et al. (2014)	 Hubble

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All areas of Fermilab science often need to create **model trained on simulated data, that also work on real detector data**!

DATASET SHIFT

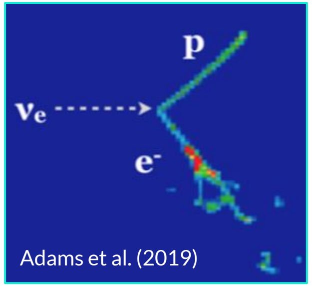
Missing and unknown physics, wrong geometry, background levels

Computational constraints for simulations

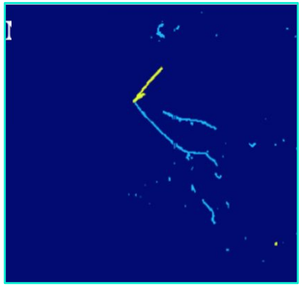
SIMULATED

REAL

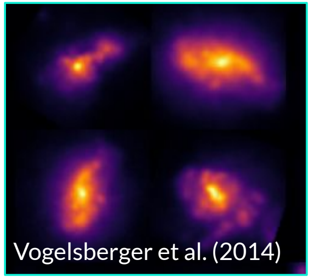
MicroBooNE (neutrinos)



Adams et al. (2019)



Illustris / Hubble (merging galaxies)


Vogelsberger et al. (2014)


Hubble

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DATASET SHIFT

- Missing and unknown physics, wrong geometry, background levels
- Computational constraints for simulations
- Detector problems, transients, errors, data compression
- Imperfect addition of observational effects

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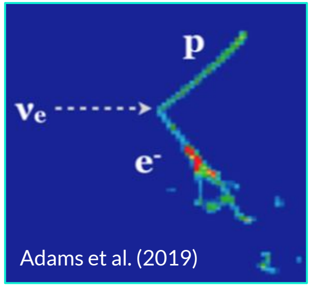
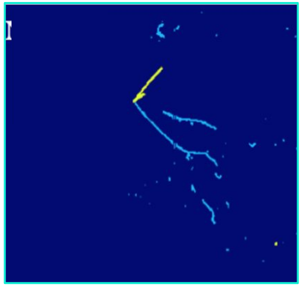
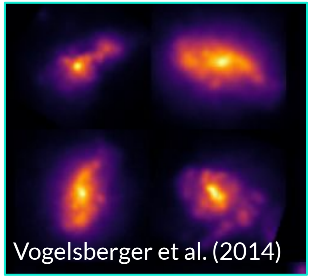
MicroBooNE (neutrinos)	 Adams et al. (2019)	
Illustris / Hubble (merging galaxies)	 Vogelsberger et al. (2014)	 Hubble

Combining Datasets

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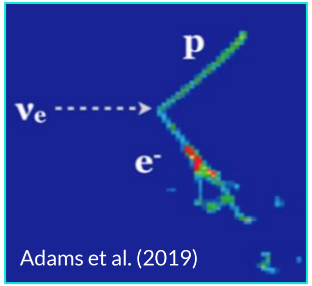
DATASET SHIFT

- Missing and unknown physics, wrong geometry, background levels
- Computational constraints for simulations
- Detector problems, transients, errors, data compression
- Imperfect addition of observational effects
- Different detectors or telescopes

SIMULATED | REAL

MicroBooNE (neutrinos)



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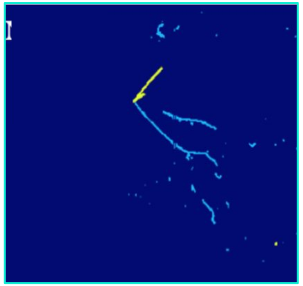

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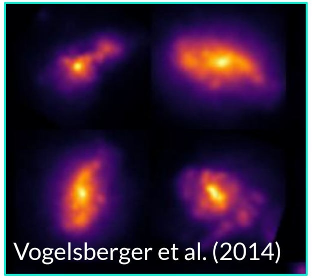
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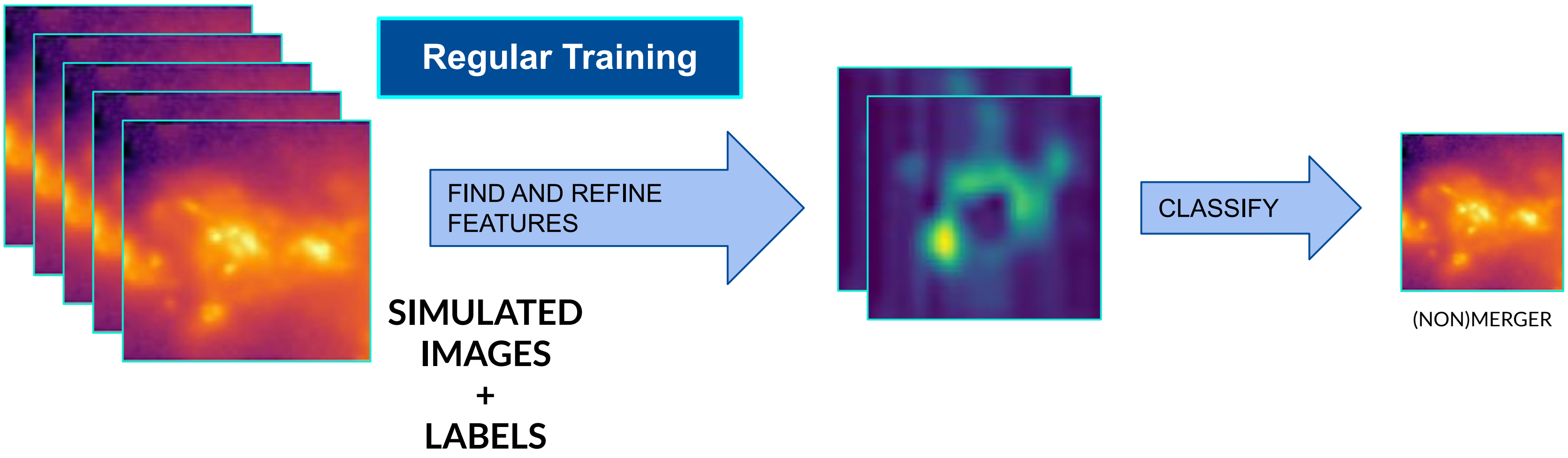
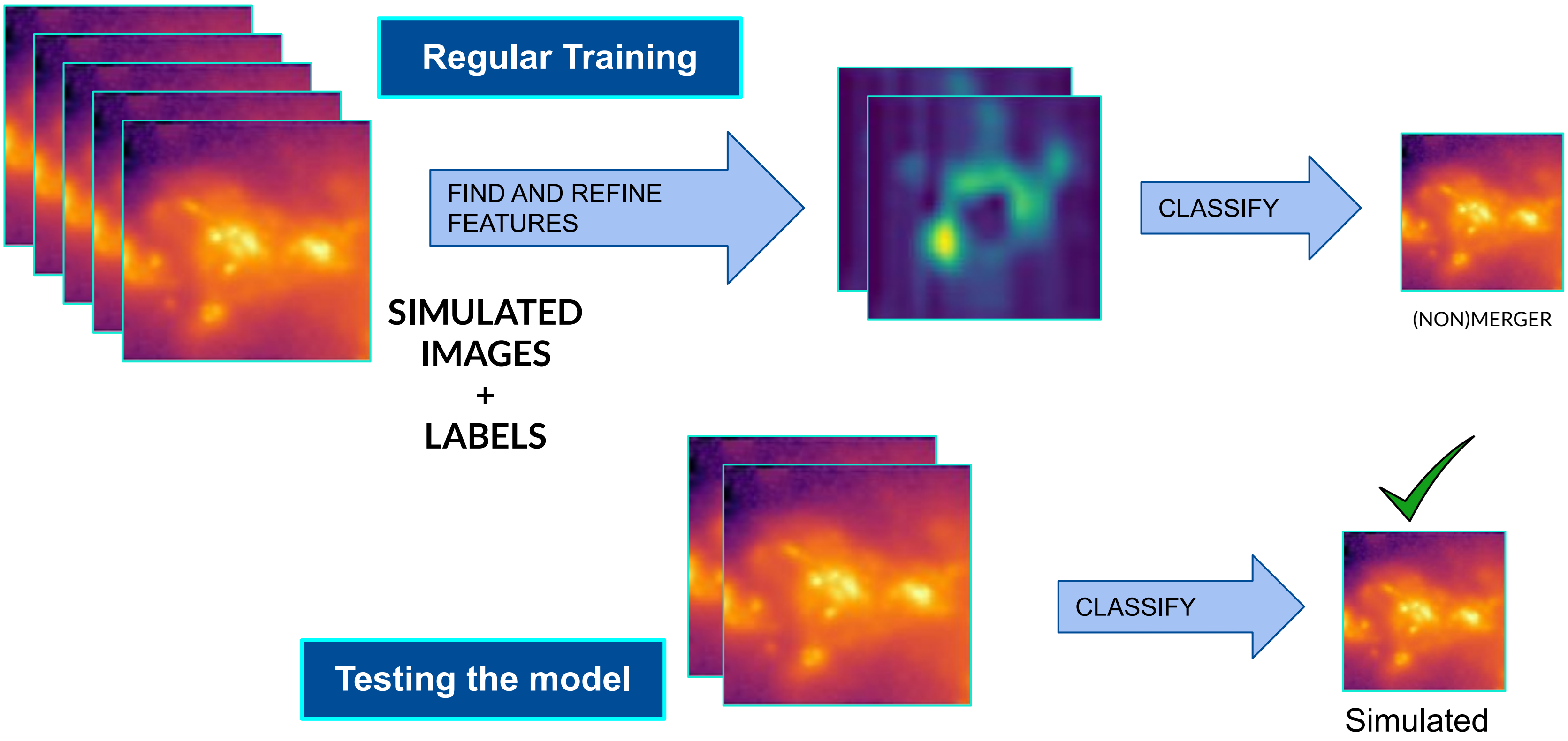
Hubble

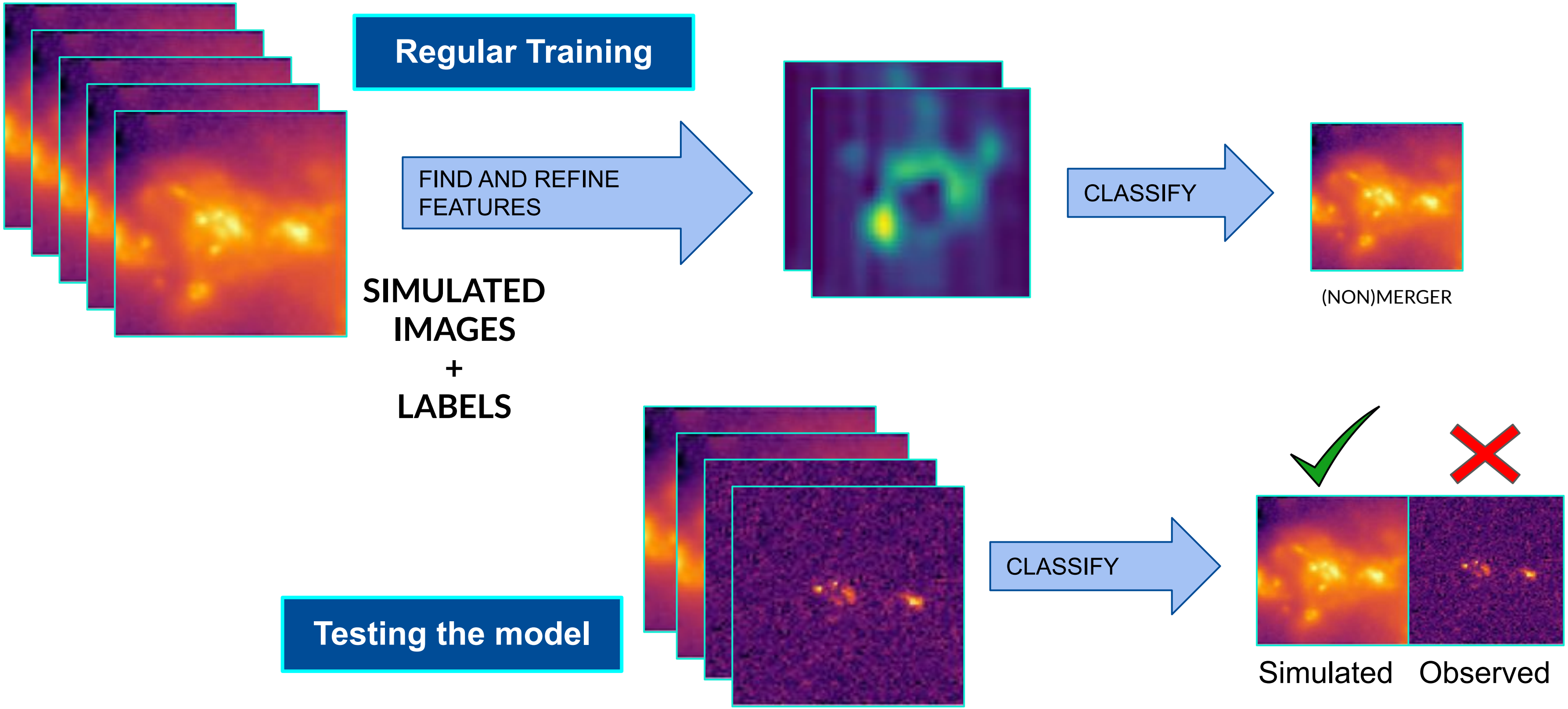
Combining Datasets



Combining Datasets



Combining Datasets



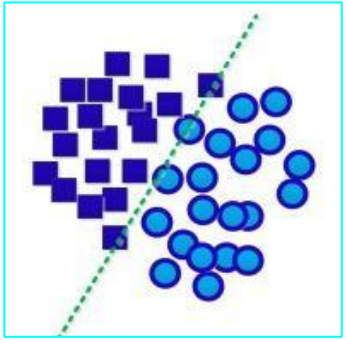
Combining Datasets

Why does this happen?

Combining Datasets

Why does this happen?

Source Domain



Train the model on source dataset and find the decision boundary.

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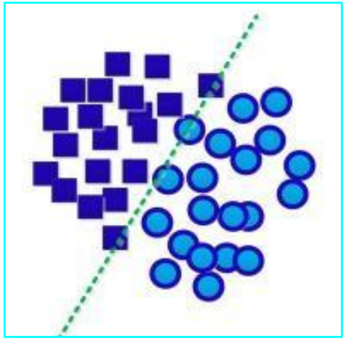
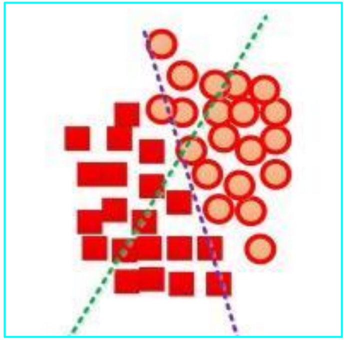
Combining Datasets

Why does this happen?

Source Domain



Target Domain



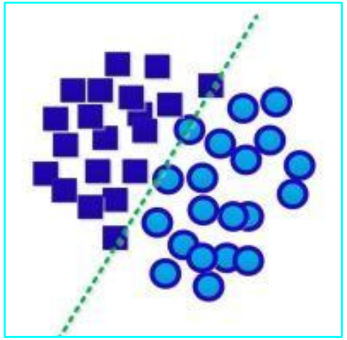
New domain is shifted, learned decision boundary doesn't work.

Combining Datasets

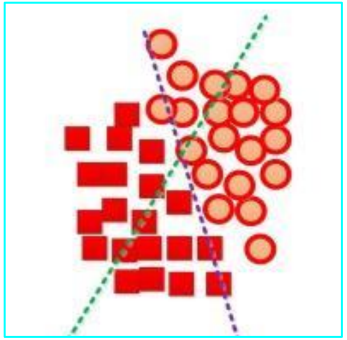
Why does this happen?

We need to align the data during training!

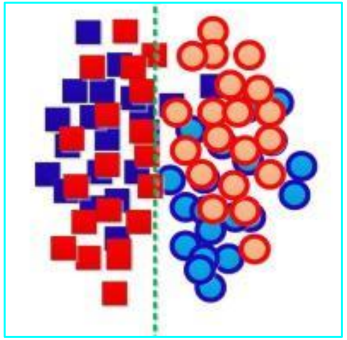
Source Domain



Target Domain



Domain Alignment



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Combining Datasets

DOMAIN ADAPTATION

Align data distributions in the latent space of the network by forcing the network to **find more robust domain-invariant features.**

Combining Datasets

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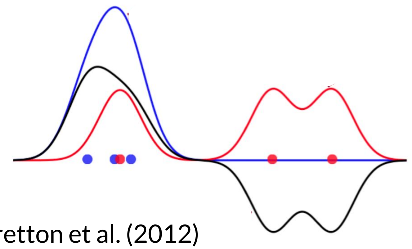
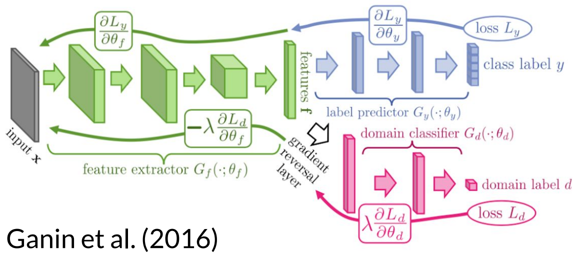
Distance-based methods

Adversarial methods



Gretton et al. (2012)



Ganin et al. (2016)

Combining Datasets

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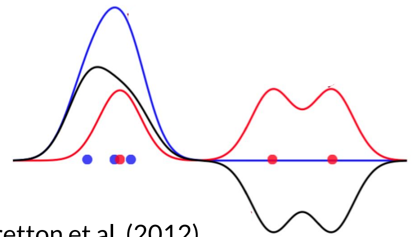
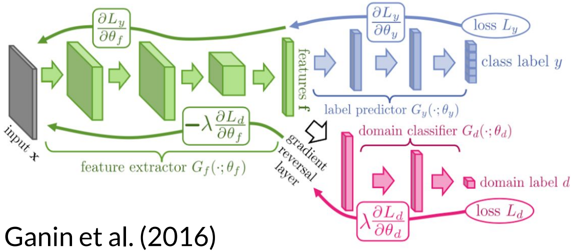


Gretton et al. (2012)

Training = Task Loss + DA Loss



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Combining Datasets

DOMAIN ADAPTATION

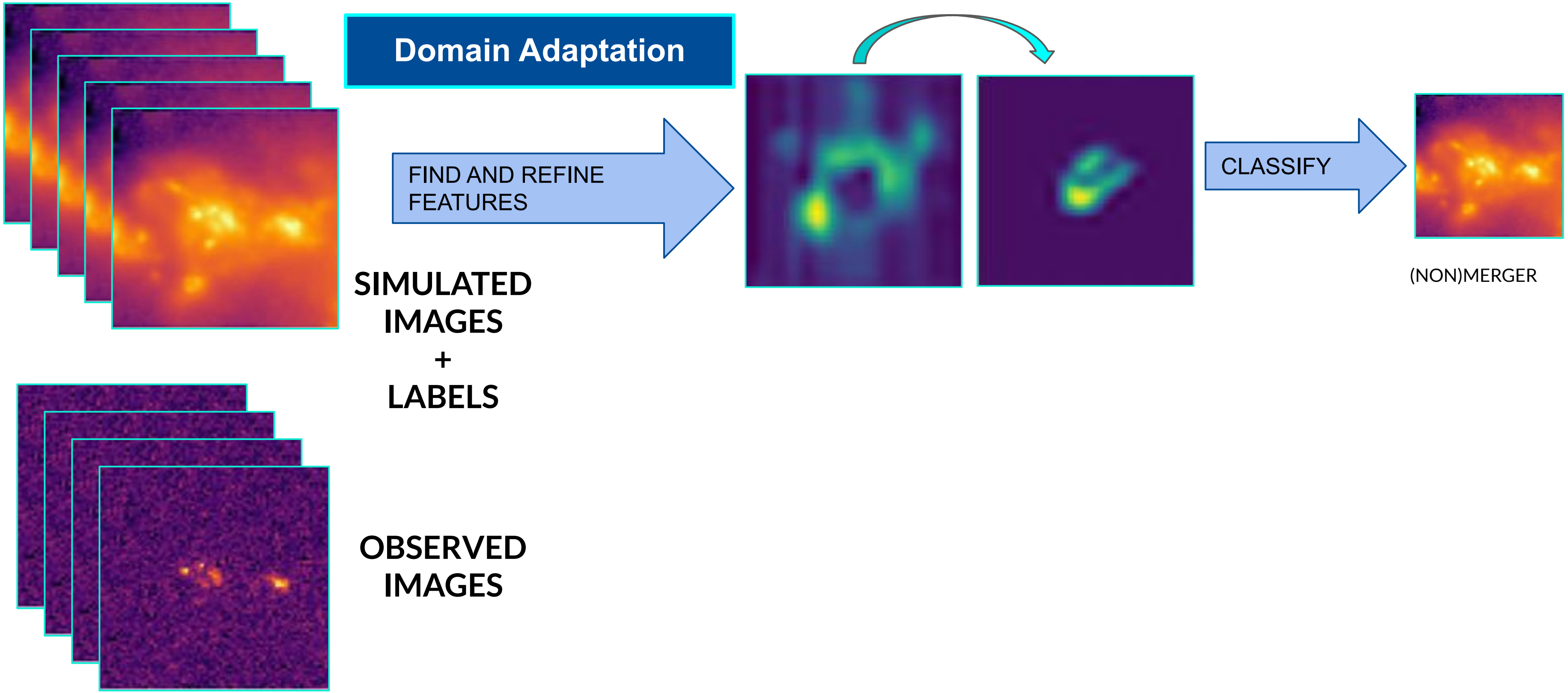
Align data distributions in the latent space of the network by forcing the network to **find more robust domain-invariant features.**

Distance-based methods

Adversarial methods

Works on **unlabeled target domain**!
Can be applied to **new data**, no need for scientists to label anythin

Combining Datasets



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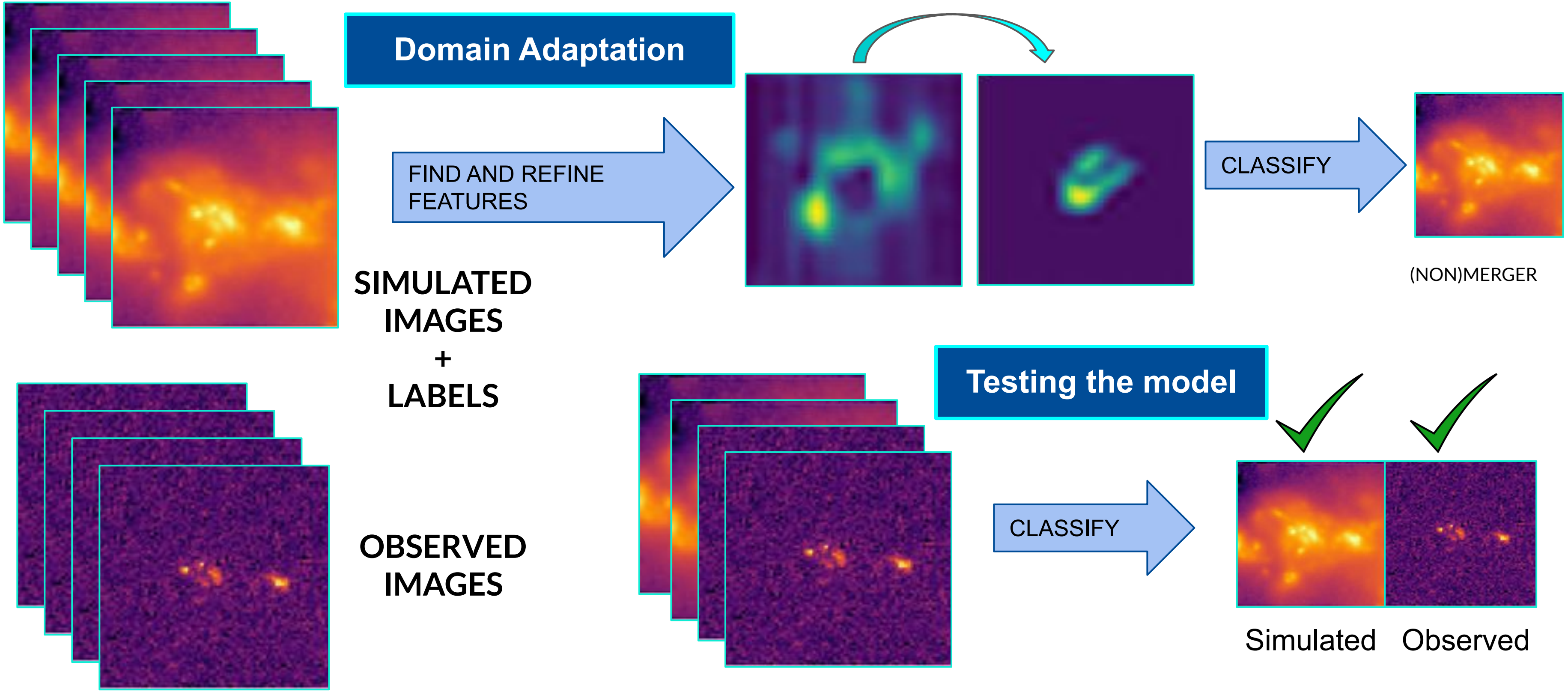
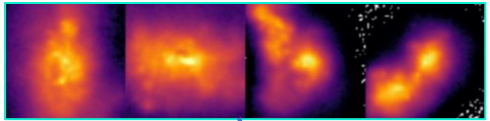
Combining Datasets

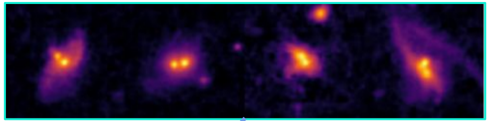


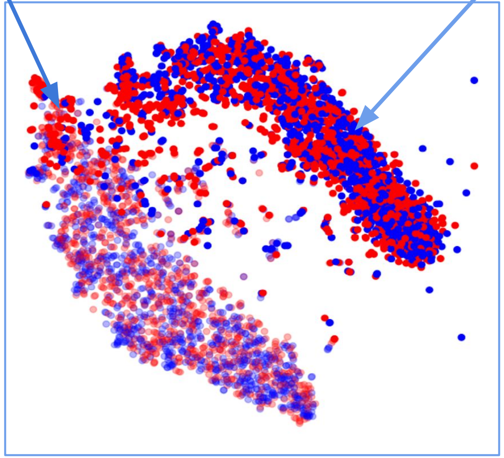
Combining Datasets

Source - Illustris



Target - SDSS observations



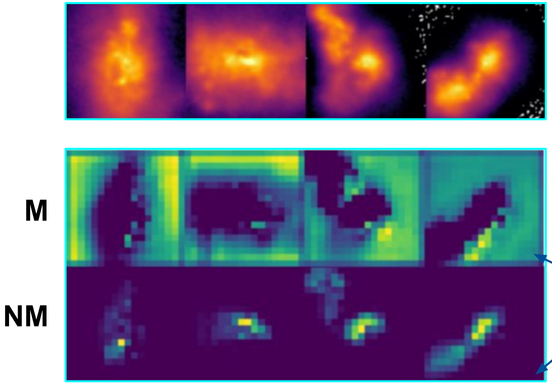


This is how the network sees the data.
2D representation of network's latent space.

Ćiprijanović et al. 2020b.
Ćiprijanović et al. 2021a.

Combining Datasets

Source - Illustris



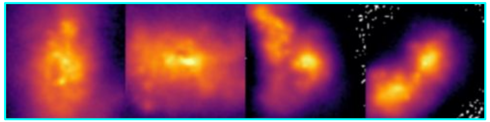
Important regions are highlighted!

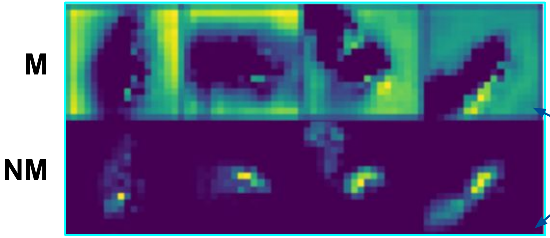
Regular Training

Ćiprijanović et al. 2020b.
Ćiprijanović et al. 202

Combining Datasets

Source - Illustris





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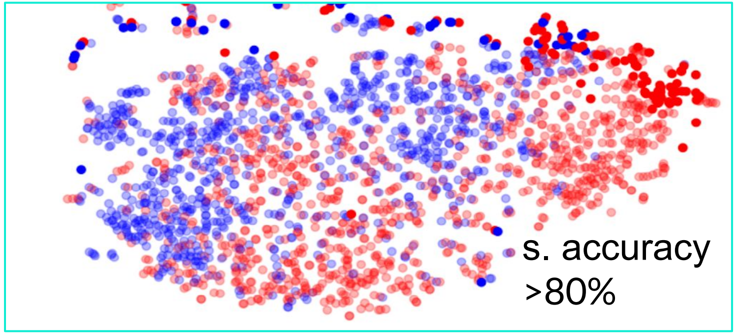
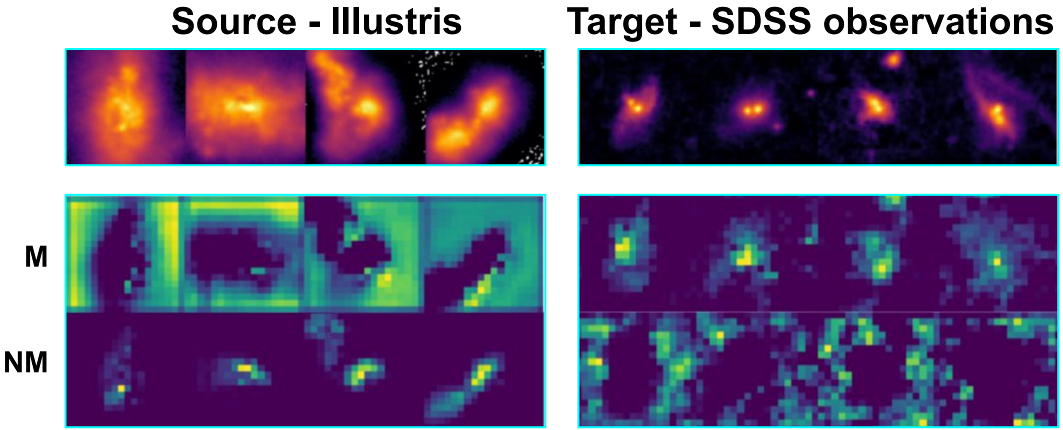


Ćiprijanović et al. 2020b.
Ćiprijanović et al. 202

Combining Datasets



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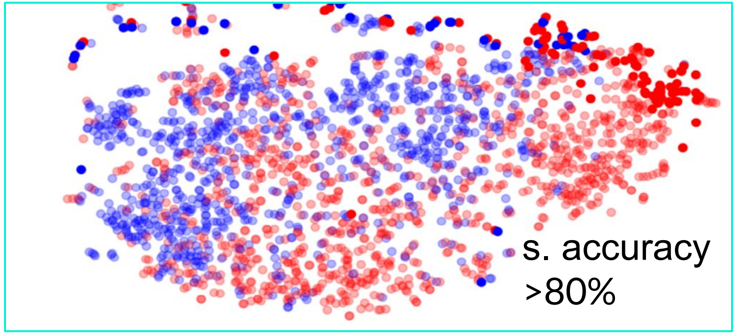

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Ćiprijanović et al. 202

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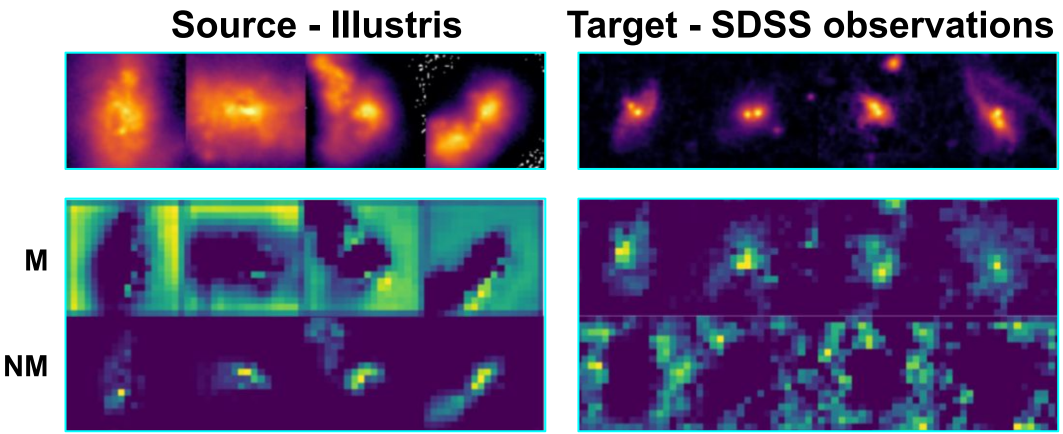

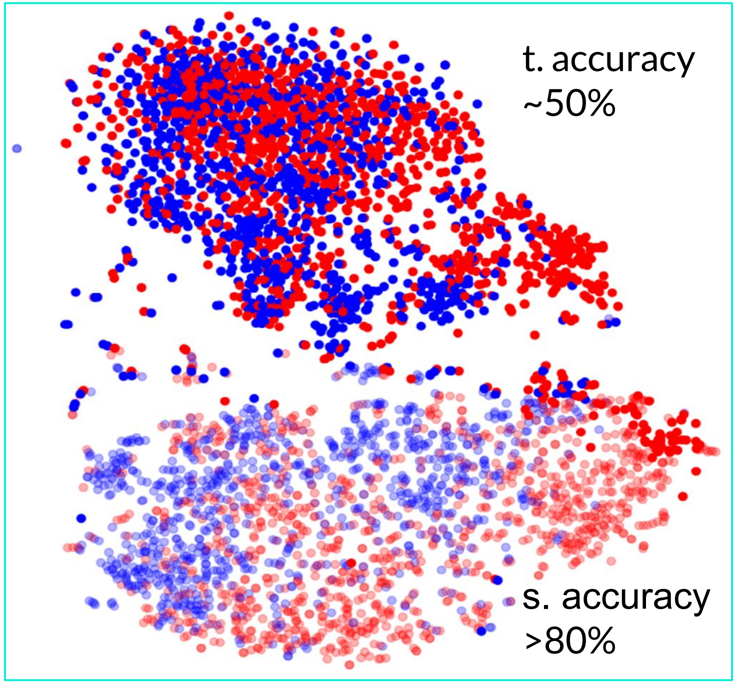

Ćiprijanović et al. 2020b.
Ćiprijanović et al. 202

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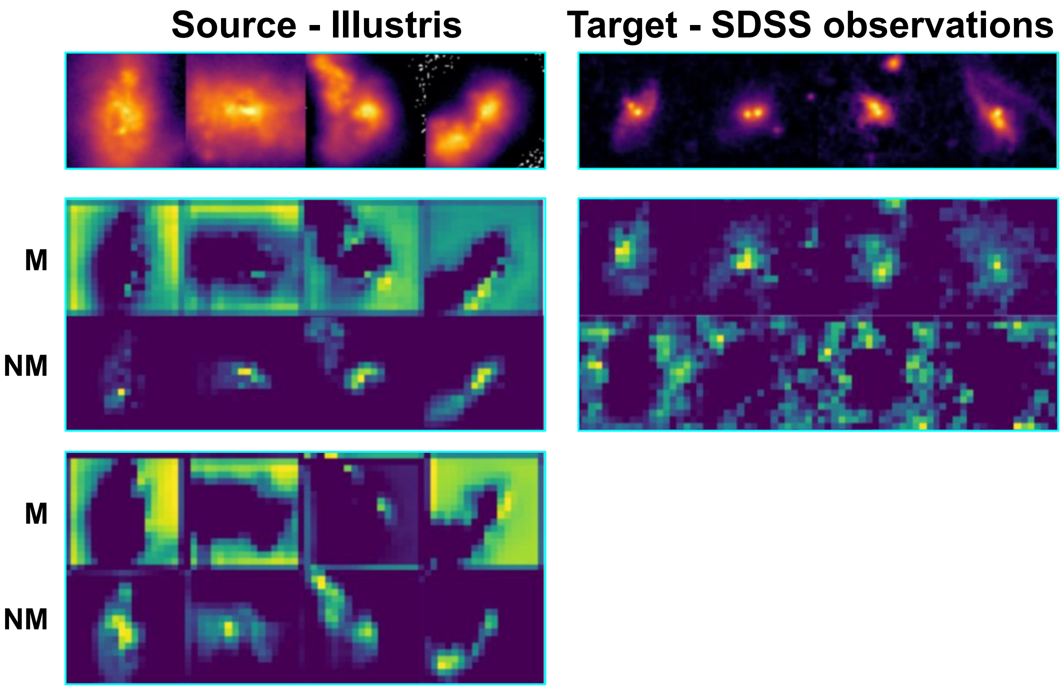
Combining Datasets



Domain Adaptation

Ćiprijanović et al. 2020b.
Ćiprijanović et al. 202

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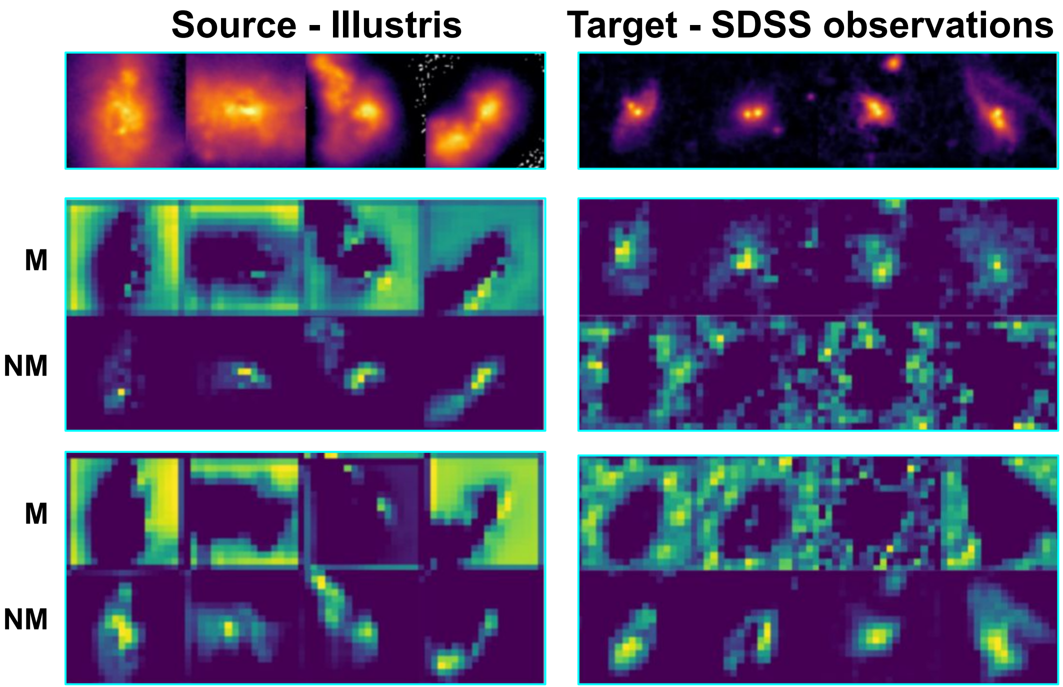
Combining Datasets



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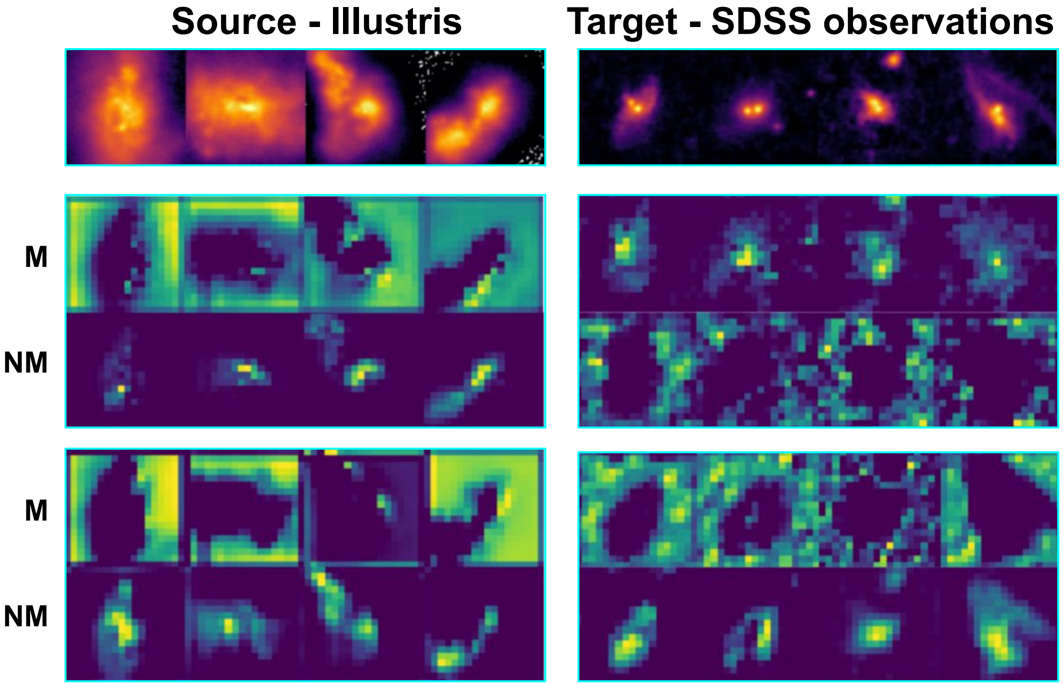
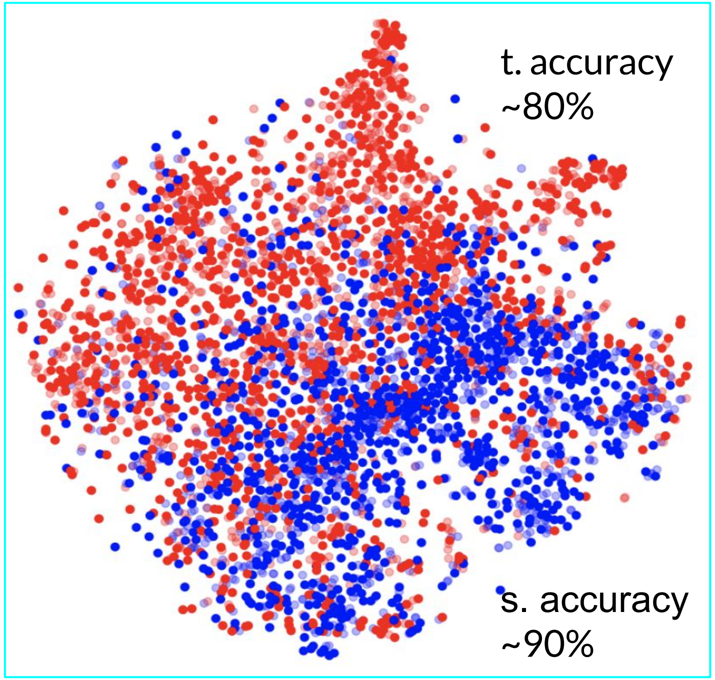


Ćiprijanović et al. 2020b.
Ćiprijanović et al. 2021a

Up to 30% increase!



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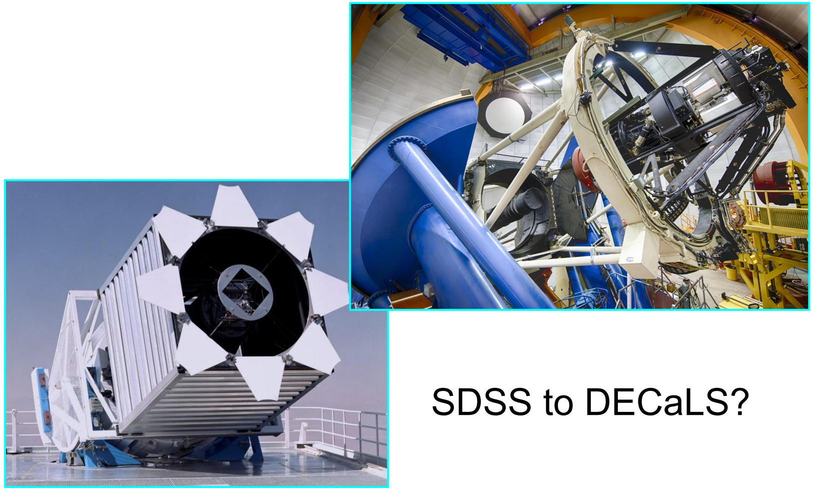
Bridging between observations - Much Harder!

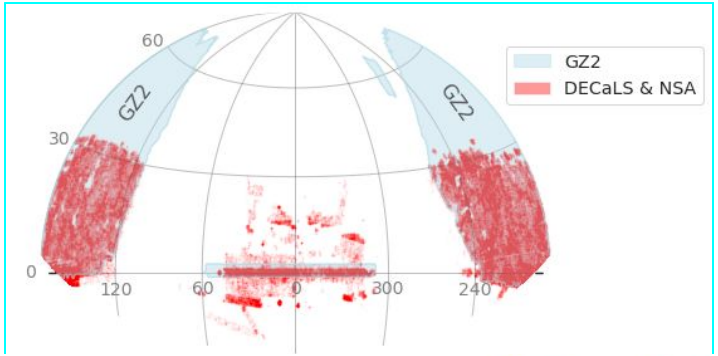
The gap between observational datasets is much larger:

- Noise, PSF
- Pixel scale
- Depth of the survey
- Magnitude limit
- Perhaps different filters
- Different data distributions….

How do we build something flexible enough to handle any kind of data distributions and distribution overlaps?



SDSS to DECaLS?



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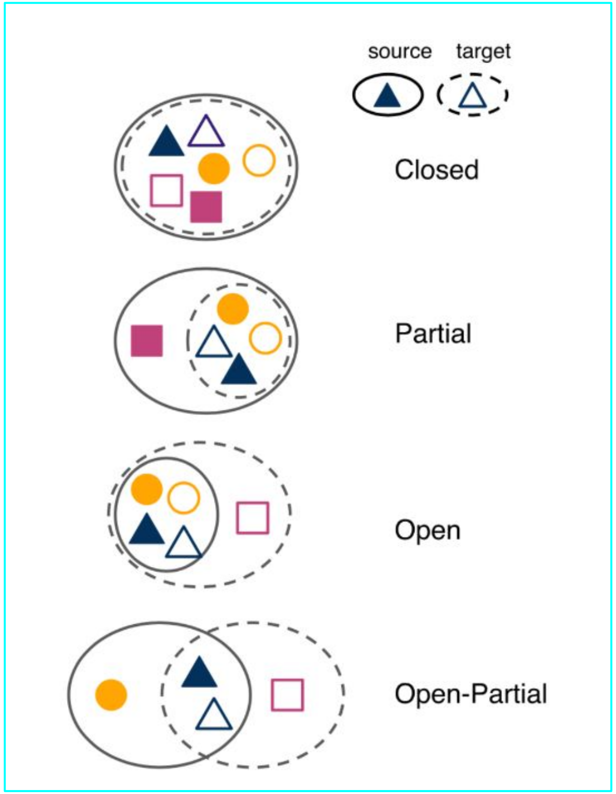
Types of Dataset Shift Problems

- Overall distribution per class can be different between datasets.
    - Overlapping classes should be aligned independently instead of aligning the entire data distribution.
- We can even have classes present in only one of the datasets - old labeled data or even new unlabeled data (so we won't even know it's there!)
    - Non-overlapping classes should not be aligned with anything.



Universal Domain Adaptation (DeepAstroUDA)

Ćiprijanović et al. 2022.
Ćiprijanović et al. 2023.

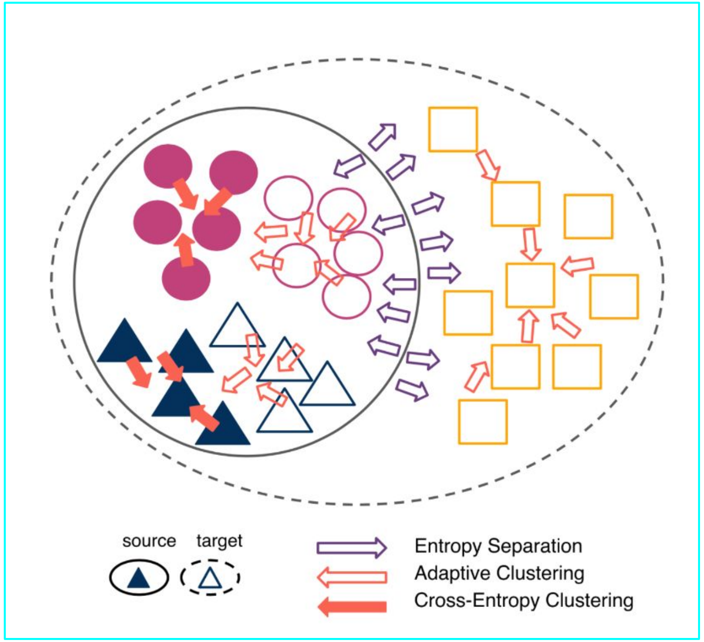
Classification of known classes

+

Clustering of similar known and unknown samples

+

Separation of different (anomalous) unknown samples



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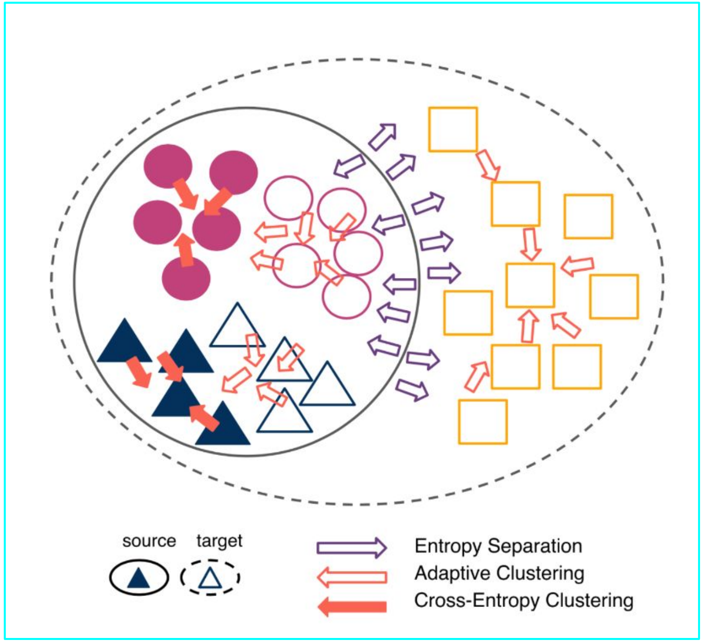


Output vector **p**

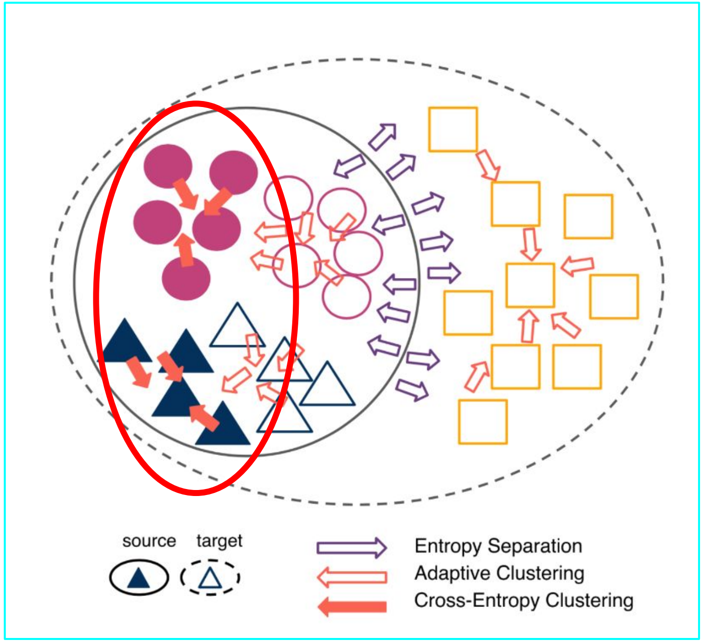
Universal Domain Adaptation (DeepAstroUDA)

Ćiprijanović et al. 2022.
Ćiprijanović et al. 2023.

Classification of known classes

$$\mathcal{L}_{\mathrm{CE}} = \frac{-\sum_{k=1}^{\mathrm{K}} w_k y_k \log \hat{y}_k}{\sum_{k=1}^{\mathrm{K}} w_k},$$

Using true and predicted labels



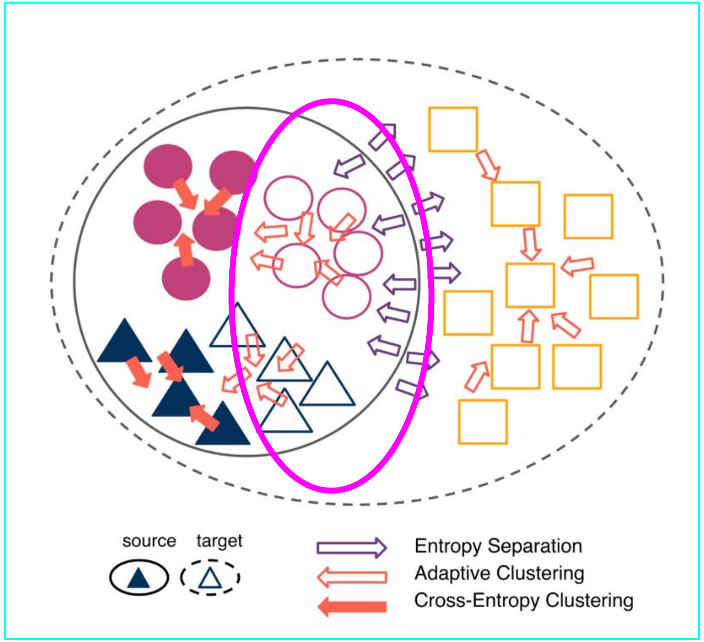
Output vector **p** → compare predicted y’ with true label y

Universal Domain Adaptation (DeepAstroUDA)

Ćiprijanović et al. 2022.
Ćiprijanović et al. 2023.

Clustering of similar known and unknown samples

Via self-supervision:
comparing pairs of output features
between all samples from both domains



0 1 2 3 4 5 6 7 8 9

Output vector **p**

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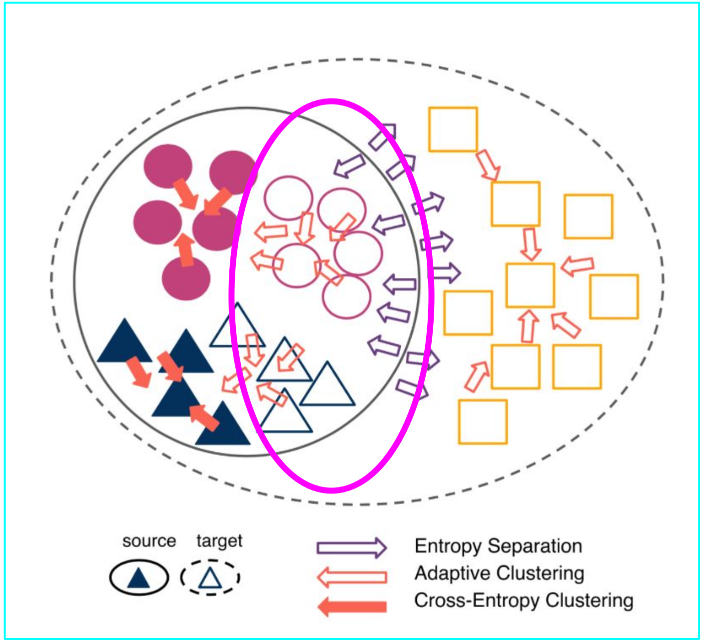
Ćiprijanović et al. 2022.
Ćiprijanović et al. 2023.

Clustering of similar known and unknown samples

Via self-supervision:
comparing pairs of output features
between all samples from both domains

$$\mathcal{L}_{\mathrm{AC}} = -\sum_{i \in B}\sum_{j \in b_t} s_{ij}\log(\mathbf{p}_i^{\top}\mathbf{p}_j) + (1-s_{ij})\log(1-\mathbf{p}_i^{\top}\mathbf{p}_j), \tag{1}$$



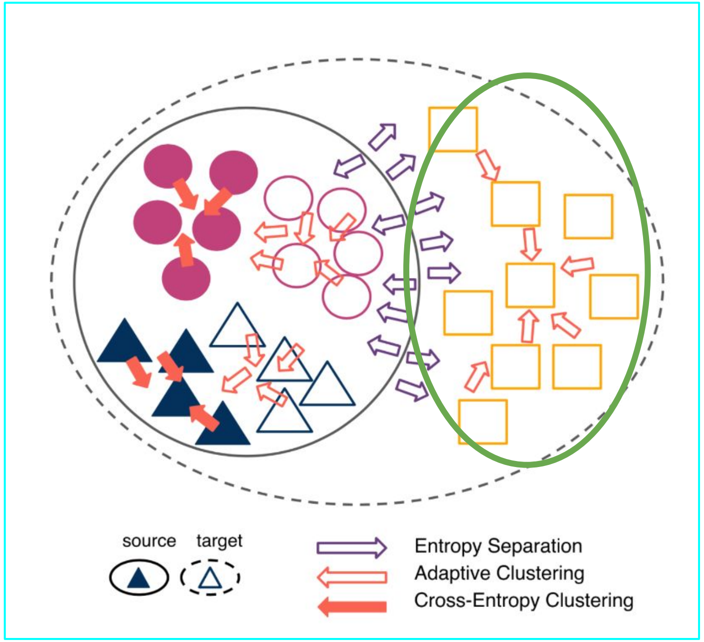
Output vector p → rank order to create similarity labels

Universal Domain Adaptation (DeepAstroUDA)

Ćiprijanović et al. 2022.
Ćiprijanović et al. 2023.

Separation of different (anomalous) unknown samples

Pushing away samples with high entropy of outputs features



0 1 2 3 4 5 6 7 8 9

Output vector p

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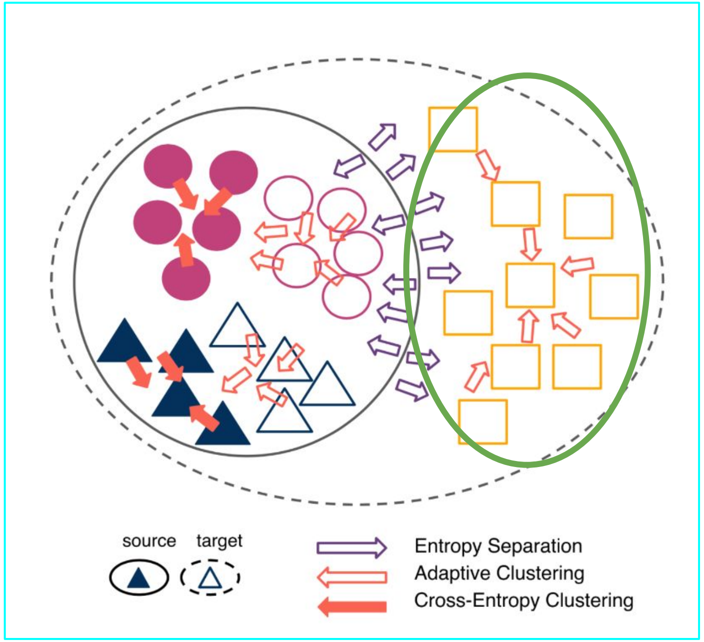
Pushing away samples with high entropy of outputs features

$$\mathcal{L}_{\mathrm{ES}}(\mathbf{p}_i) = \begin{cases} -|H(\mathbf{p}_i) - \rho| & |H(\mathbf{p}_i) - \rho| > m, \\ 0 & \text{otherwise.} \end{cases}$$

$$\mathcal{L}_{\mathrm{ES}} = \frac{1}{|b_t|} \sum_{i \in b_t} \mathcal{L}_{\mathrm{ES}}(\mathbf{p}_i).$$

$$H(X) = -\sum_{x \in X} p(x) \log p(x)$$



0 1 2 3 4 5 6 7 8 9

Output vector p → calculate entropy of each output

Universal Domain Adaptation (DeepAstroUDA)

Ćiprijanović et al. 2022.
Ćiprijanović et al. 2023.

Separation of different (anomalous) unknown samples

Pushing away samples with high entropy of outputs features

$$\mathcal{L}_{\mathrm{ES}}(\mathbf{p}_i) = \begin{cases} -|H(\mathbf{p}_i) - \rho| & |H(\mathbf{p}_i) - \rho| > m, \\ 0 & \text{otherwise.} \end{cases}$$

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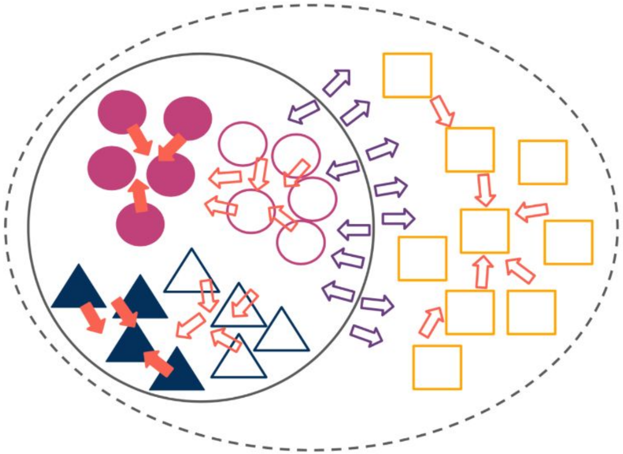

$$\mathcal{L} = \mathcal{L}_{CE} + \lambda(\mathcal{L}_{\mathrm{AC}} + \mathcal{L}_{\mathrm{ES}}).$$

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Output vector p → calculate entropy of each output

Universal Domain Adaptation (DeepAstroUDA)

DA tests we ran:

- Two data releases from the same telescope
  - LSST mocks Y1 and Y10
- Different surveys
  - SDSS and DECaLS
- Wide and deep fields in the same survey
  - SDSS wide and Stripe 82 deep field

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Class labels are from Galaxy Zoo 2 & 3 (crowdsourcing labels ~10^5 volunteers).

Known classes:
Disturbed (0)
Merging (1)
Round smooth (2)
Cigar shaped smooth (3)
Barred spiral (4)
Unbarred tight spiral (5),
Unbarred loose spiral (6)
Edge-on without bulge (7),
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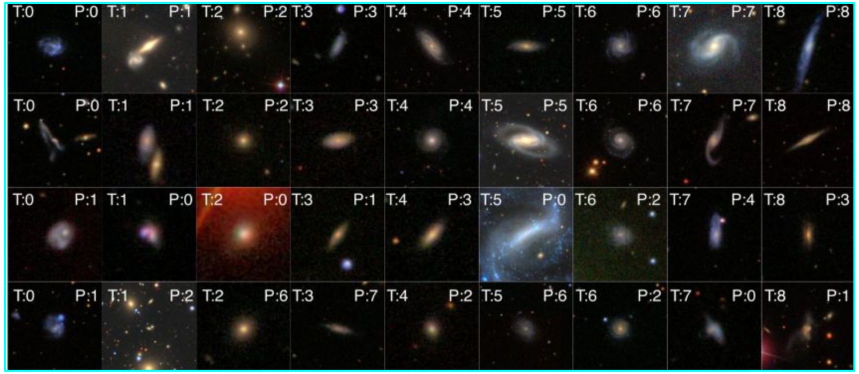
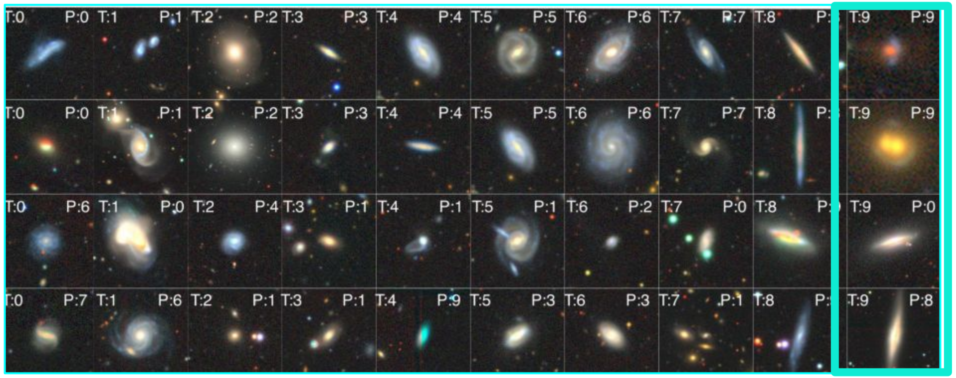
Unknown anomaly class (only in DECaLS):
Strong gravitational lens (9)

Universal Domain Adaptation (DeepAstroUDA)

SDSS



DECaLS



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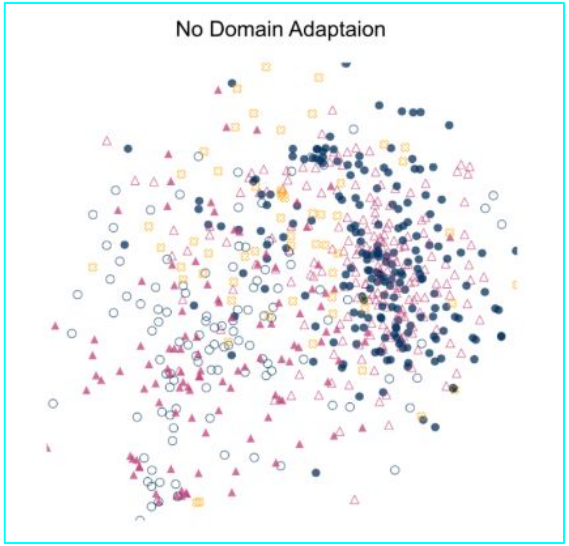
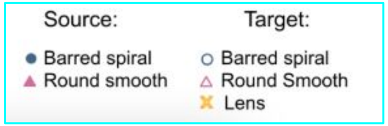


Classes are mixed!



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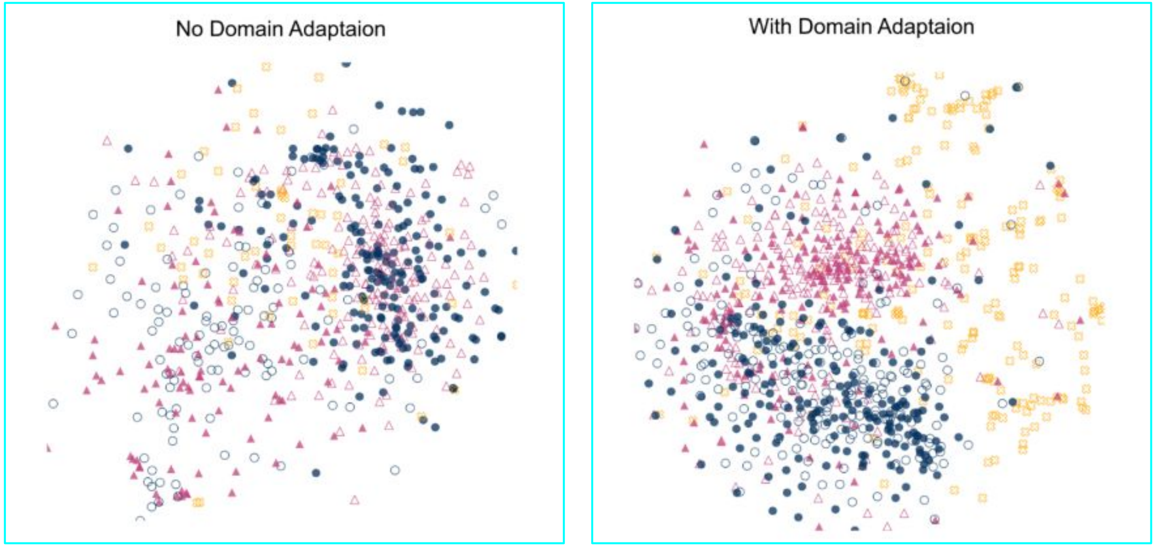

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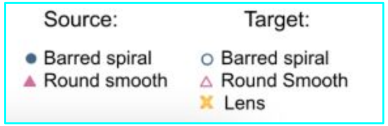
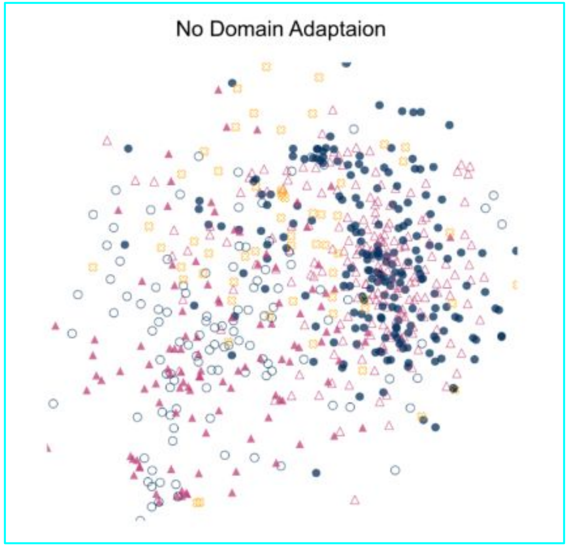
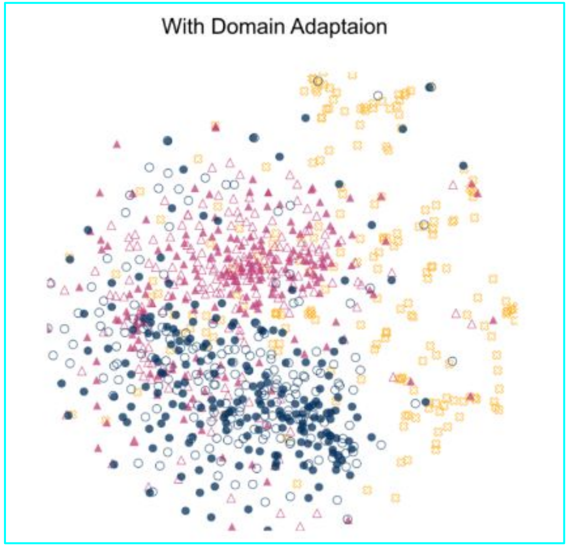
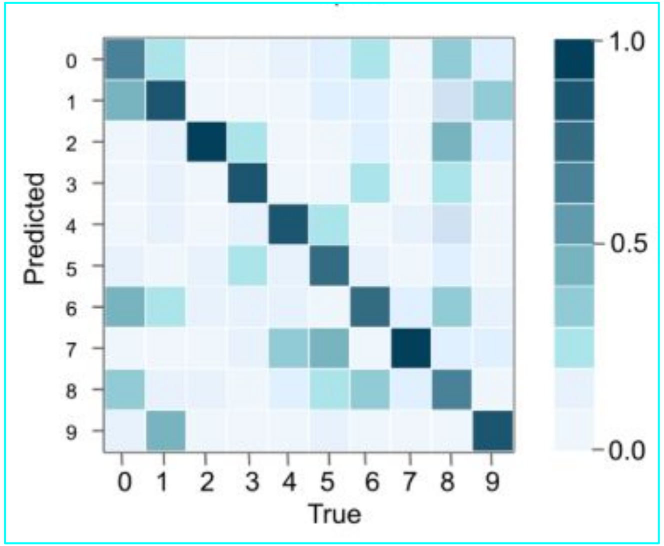


Known classes overlap,
unknown is pushed to the side.

Universal Domain Adaptation (DeepAstroUDA)







Classes are mixed!

Source:	Target:
● Barred spiral	○ Barred spiral
▲ Round smooth	△ Round Smooth
	✕ Lens

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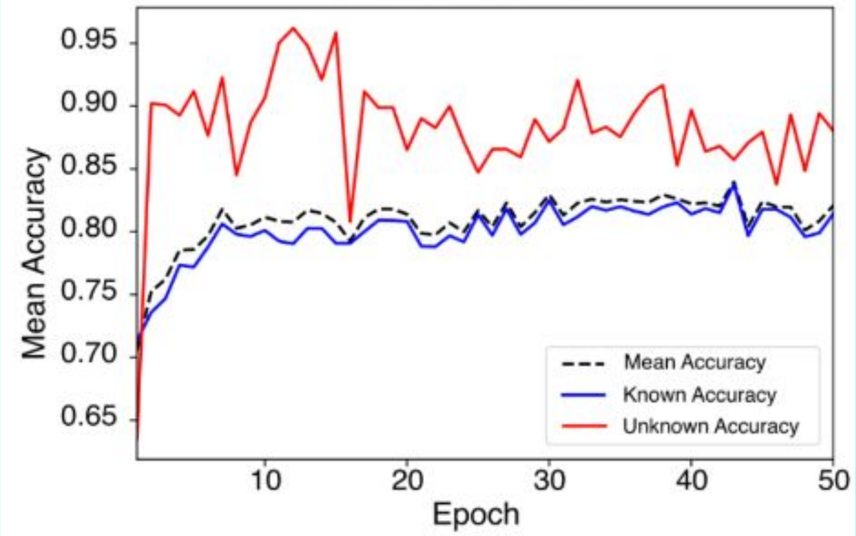
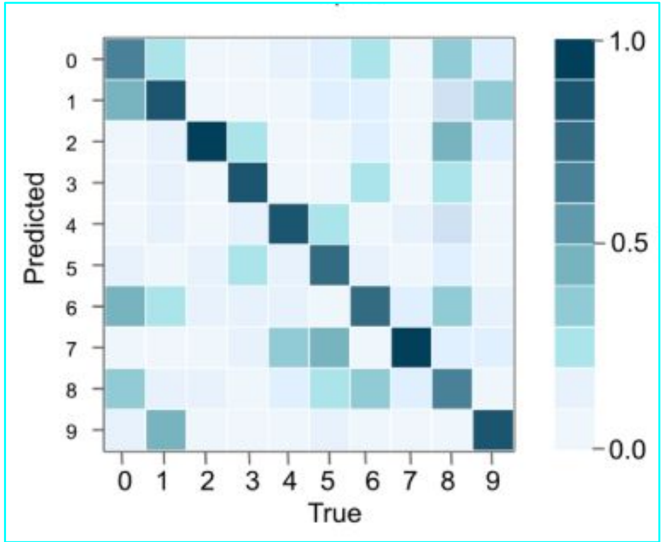
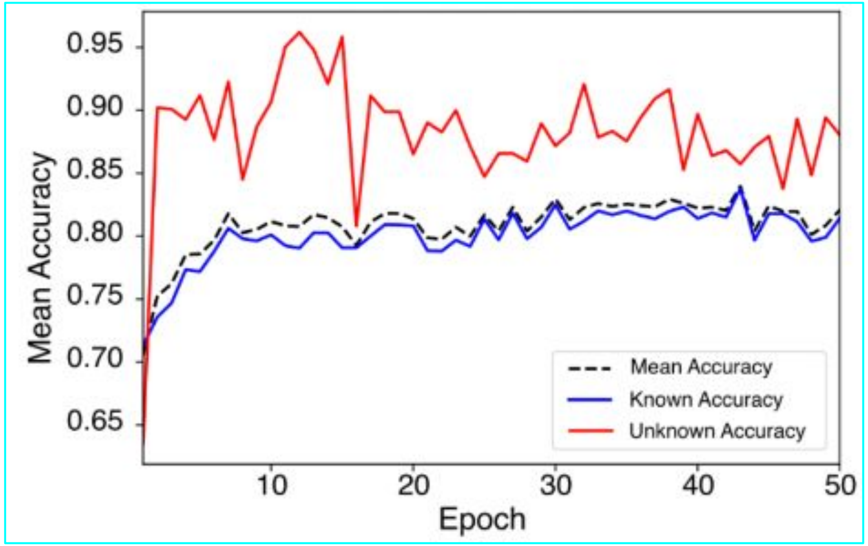


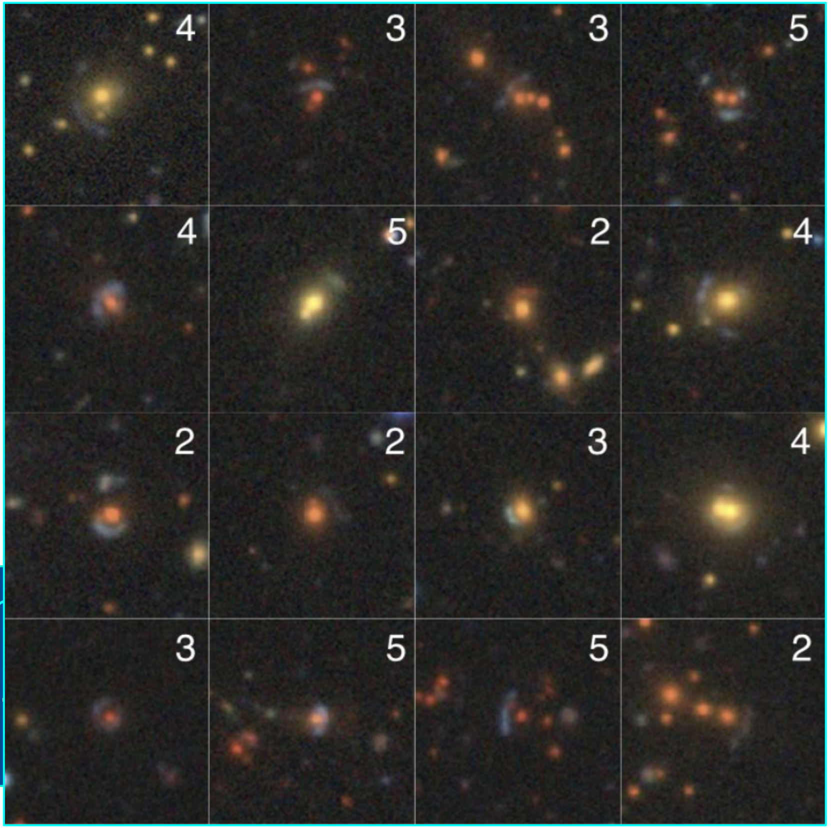


- Most confusion between classes is for truly morphologically similar classes, like disturbed and merging.
- Model is very sure about the unknown lens class - it can recognize these object look different than all other known classes.

Fermilab

Universal Domain Adaptation (DeepAstroUDA)





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Talk Outline

1. Domain Shift Problems

2. Domain Adaptation

3. Universal Domain Adaptation

4. Future Challenges

- Simulation and observations

Ćiprijanović et al. 2021.

- Increase robustness to data perturbations

Ćiprijanović et al. 2022.

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Ćiprijanović et al. 2022.
Ćiprijanović et al. 2023.

FUTURE CHALLENGES

- Connecting extracted features to physical properties.
- Guiding the model to use some preferred physical features and discover the rest.
- Understanding and exploring the latent space.
- Can we get any new insights from AI?
- What if the domain shift is physical not instrumental/computational?

Big thanks to all my amazing collaborators

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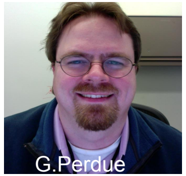
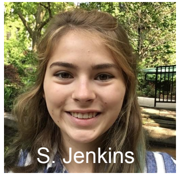
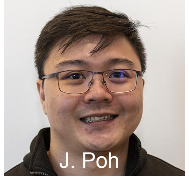
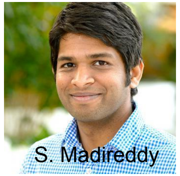


University of Chicago



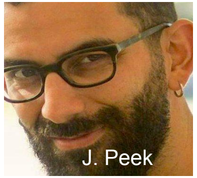


Argonne, Oakridge



and many more!

Space Telescope Science Institute



THE UNIVERSITY OF CHICAGO 1890

Argonne NATIONAL LABORATORY

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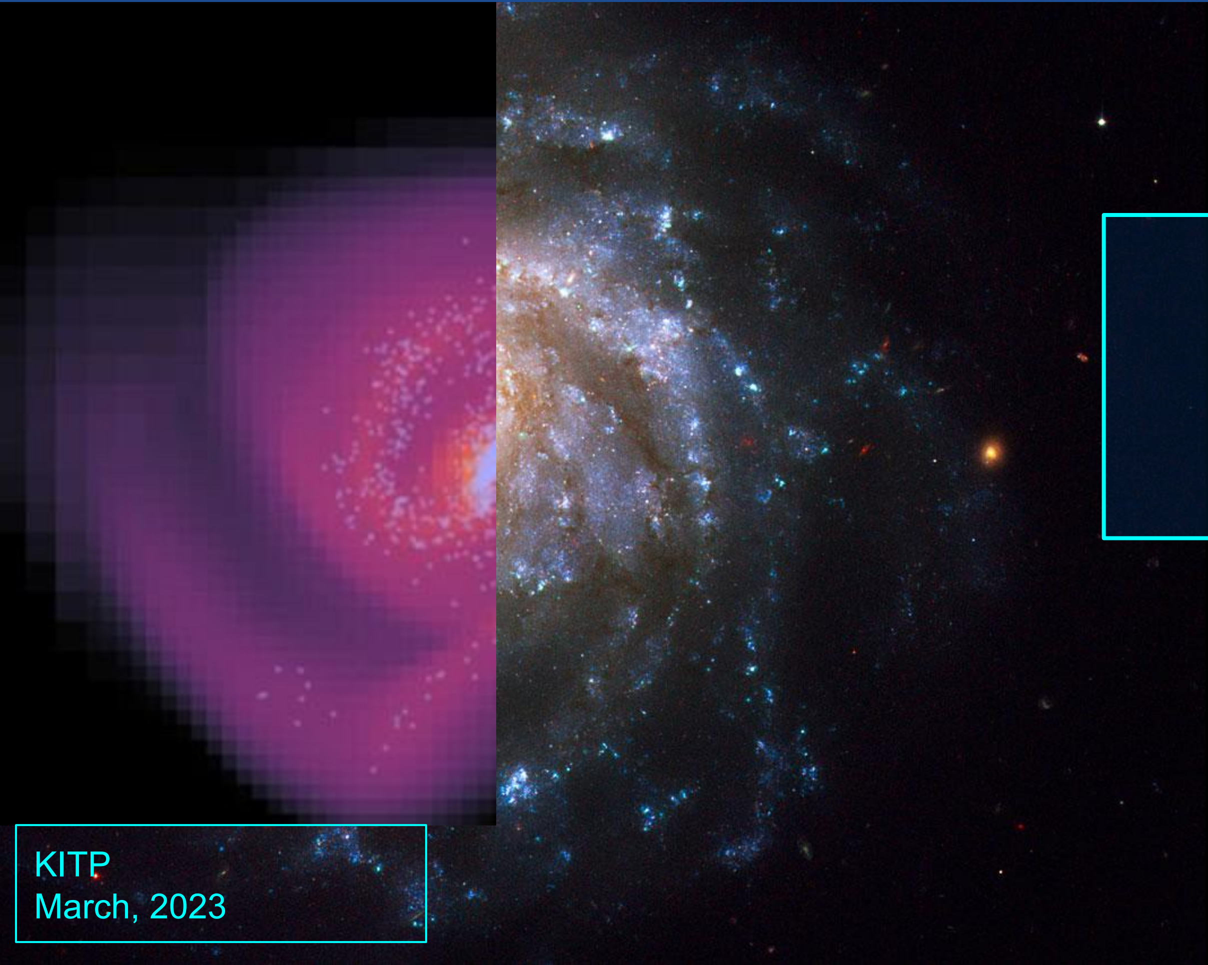

THANK YOU!

KITP
March, 2023

Aleksandra Ćiprijanović
(she/her/hers)

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aleksand@fnal.gov