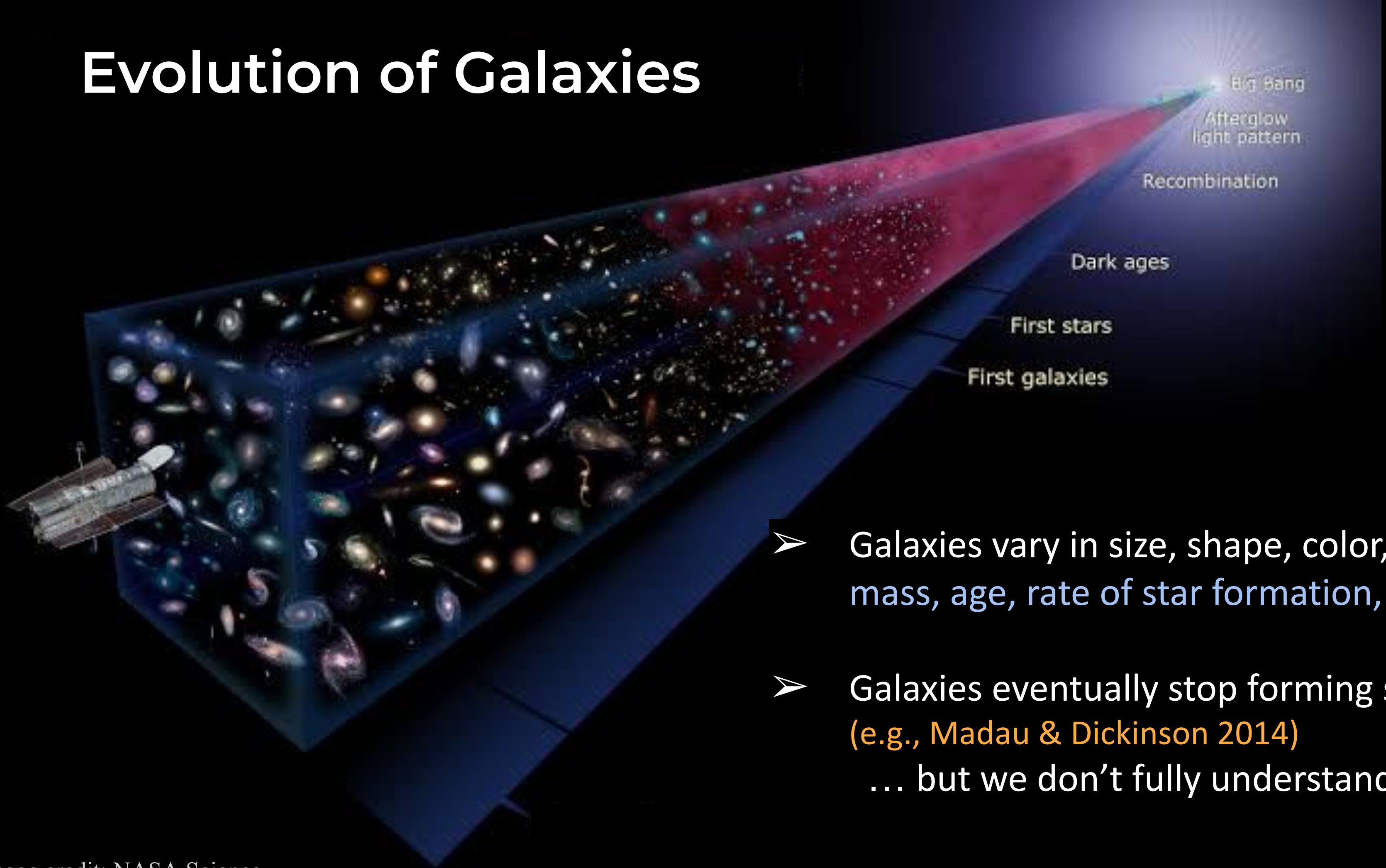
What is ML *really learning* from galaxy spectra?

Stéphanie Juneau
NOIRLab

Collaborators: Felix Pat, Isabella Olin, Christina Williams, Andy Morgan (NSF NOIRLab), Yufeng Luo, Adam Myers (Wyoming), Adam Bolton (SLAC), Dalya Baron (Stanford), Vanessa Böhm, Alex Kim (Berkeley), NSF-Simons CosmicAI institute

ESA/Hubble & NASA

Evolution of Galaxies

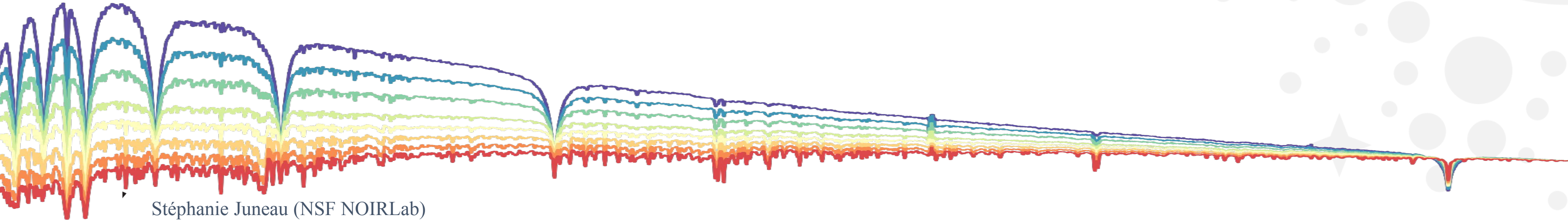


- Galaxies vary in size, shape, color, mass, age, rate of star formation, etc.
- Galaxies eventually stop forming stars (e.g., Madau & Dickinson 2014)
  … but we don't fully understand why

Image credit: NASA Science

Optical spectra encode astrophysics

- **Galaxy spectra contain *a lot of information*** (stellar population age, mass, star formation rate, gas kinematics, etc.) but are **difficult to interpret** due to degeneracies between spectral features and underlying physics



Stéphanie Juneau (NSF NOIRLab)

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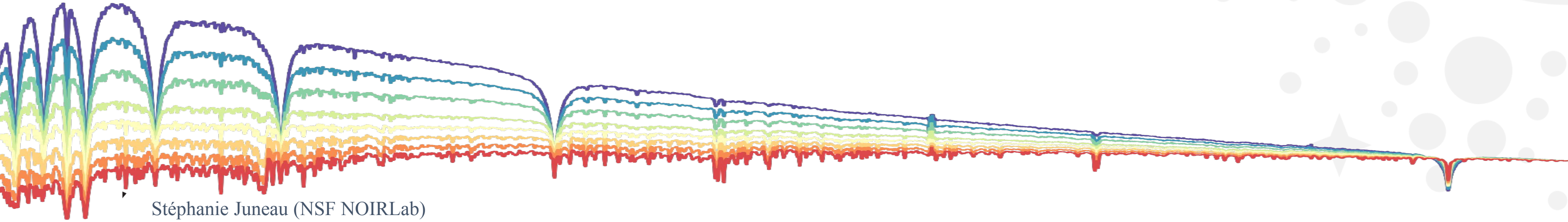
- Part I: Apply **machine learning methods** to:
  - Decrease the complexity & sort the information from a large number of spectra
  - Reveal trends or classification based on the entire spectra



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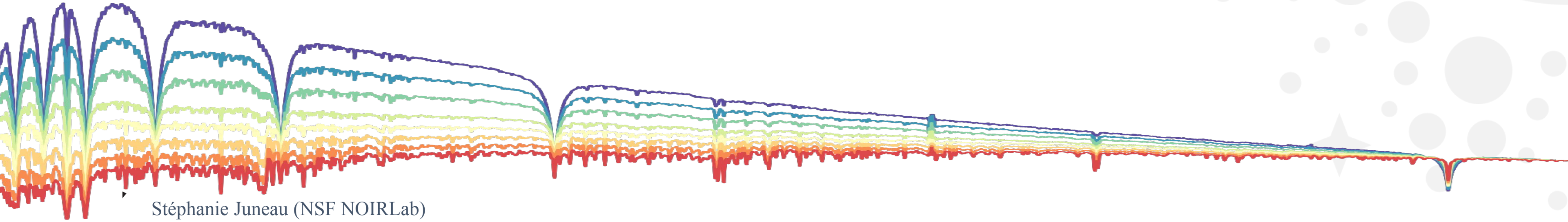
- Part II: Revert to astrophysical galaxy property studies for **interpretability**:
  - Understand what features and trends the models / latent space identified
  - Inform future experiments



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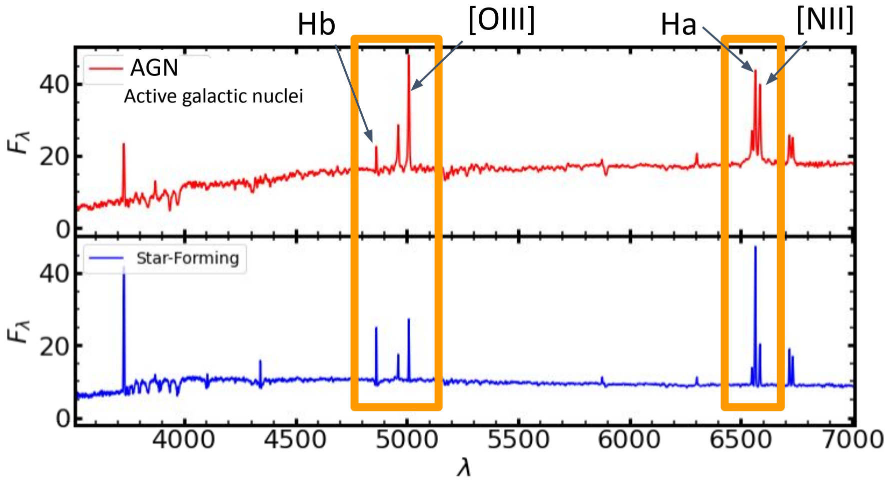
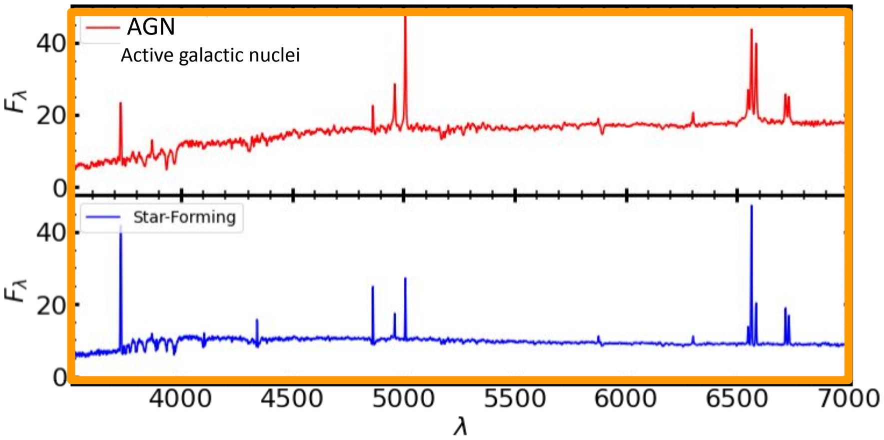
Using ML to Extract information from spectra

- Principal Component Analysis (**PCA**; e.g., Boroson+03, 04, Rogers+07, McGurk+10)
- Variational Autoencoders (**VAE**; Portillo+20, Nicolaou+25)
- Probabilistic Variational Autoencoders (**PAE**; Pat, SJ+22, Melchior+23, Böhm+23, Liang+23a, 23b)

*+ see talks by **Andy Morgan** (today), **Yufeng Luo** (Wed) for foundation models using spectra*

Example: moving from using emission lines (line ratios) to the full spectral range





Probabilistic Autoencoder (PAE)

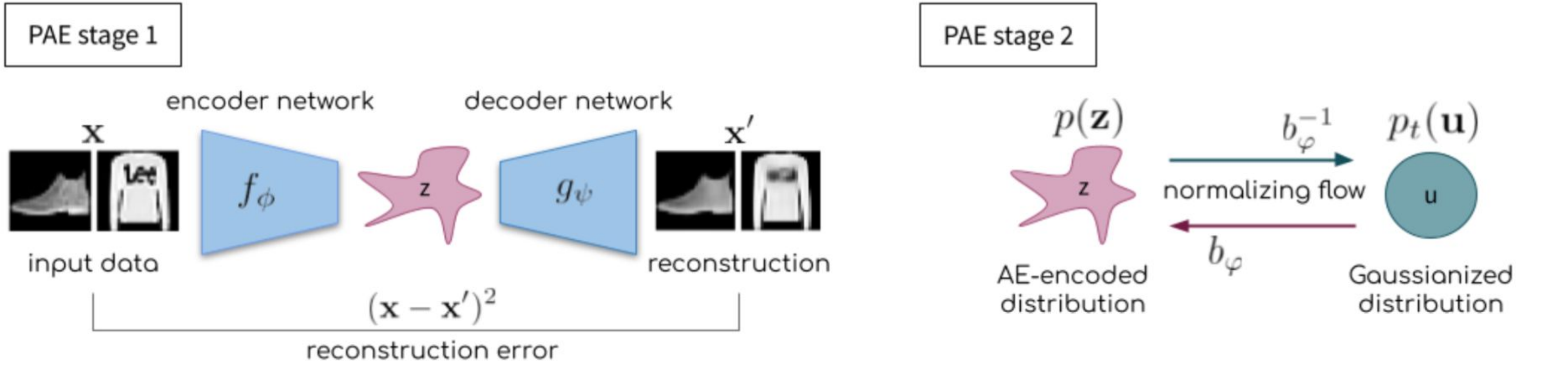


Figure 1. The two-step training of a Probabilistic Autoencoder (PAE) illustrated on an image data set. In the first stage, an autoencoder (AE) consisting of two neural networks is trained to minimize the reconstruction error after compressing (encoding) the data in a lower-dimensional latent space and decompressing (decoding) it back into the high-dimensional data space. In the second stage, a normalizing flow (NF) is trained to learn a bijective mapping from the AE-encoded latent space to a space in which the encoded data follows a Gaussian distribution.

github.com/VMBoehm/PytorchPAE

(Böhm & Seljak 2022; Böhm, Kim & Juneau 2023)

SDSS galaxy spectra → 2D projection

Classes
- Star Forming
- Composite
- Narrow-Line AGN
- Broad-Line
- Retired
- Passive

Goal: Search for astrophysical trends based on full spectra processed with machine learning

Method: Prototype work with ~209,462 SDSS spectra (Pat, SJ et al. 2022; arXiv:2211.11783)

- Spectra in rest-frame (1000D)
- Encode in 10D with Autoencoder (unsupervised; Böhm+2023)
- Project to 2D with UMAP
- Color-code galaxies with traditional classification

SDSS-IV supported by Alfred P. Sloan foundation, U.S. Dept of Energy Office of Science and the Participating Institutions: sdss4.org

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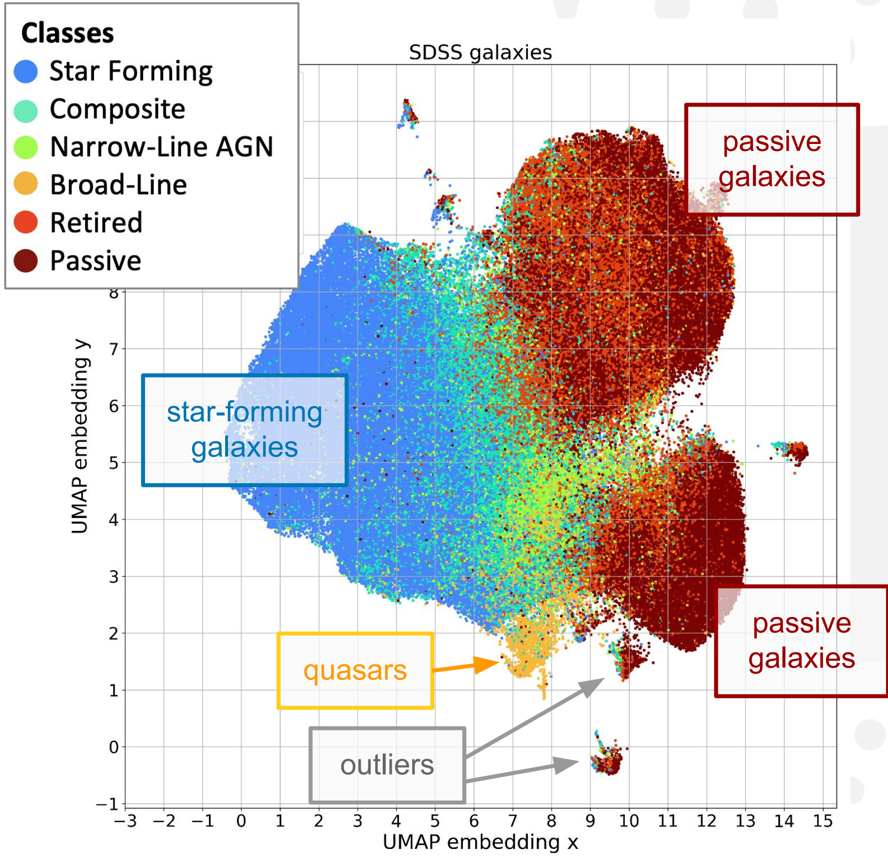

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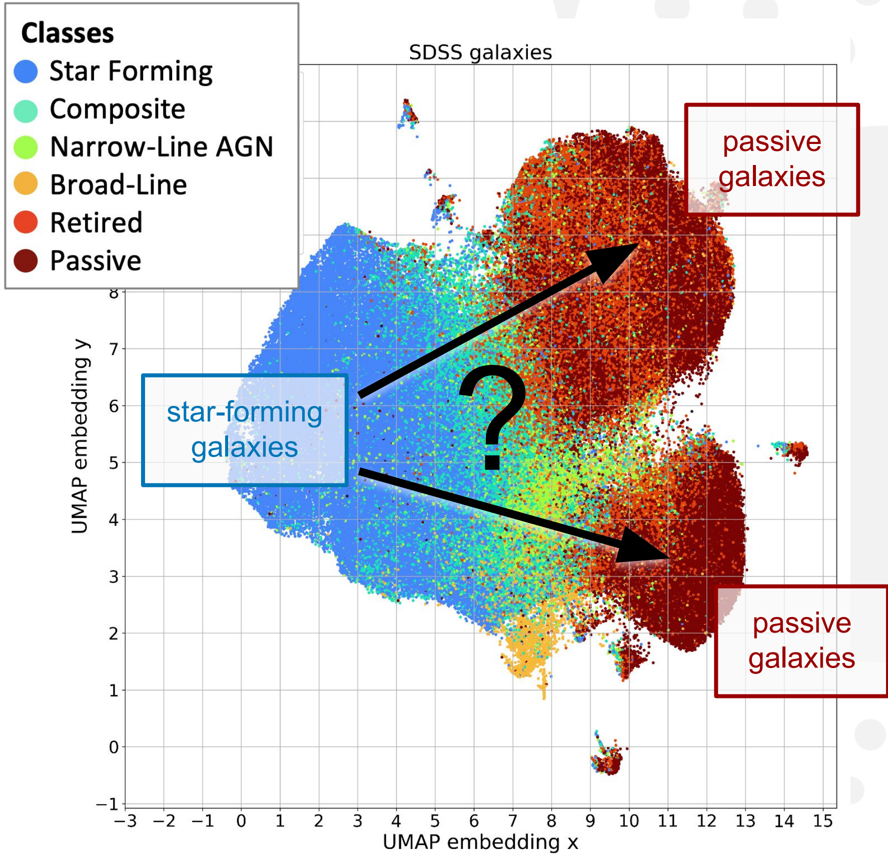
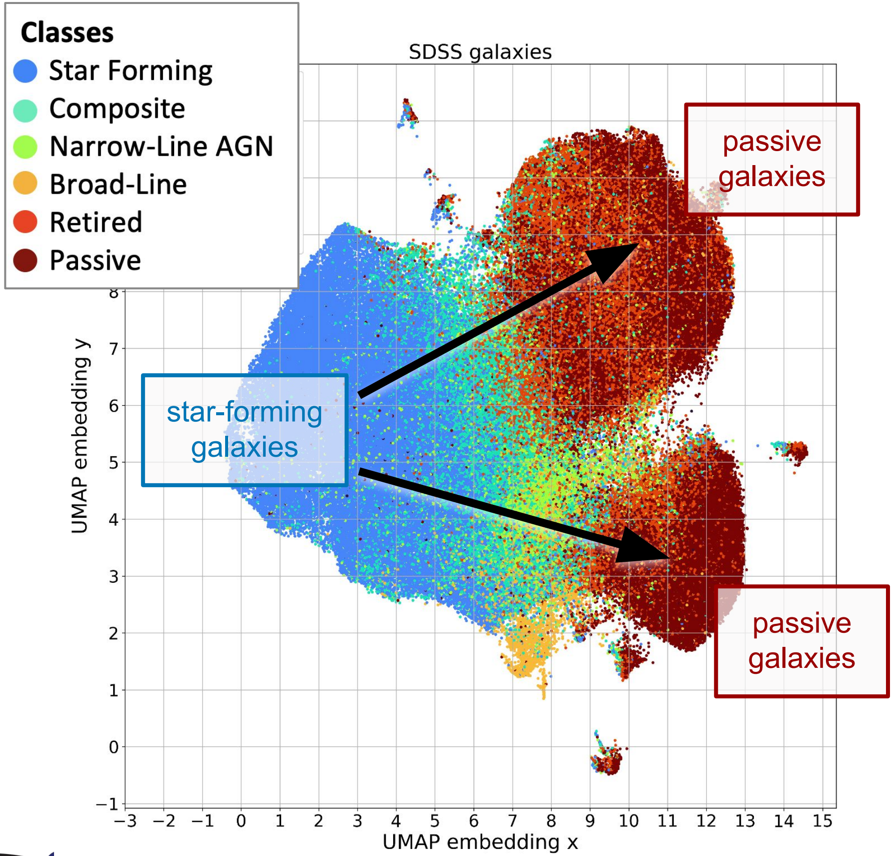
Result: Possible gradients from **star-forming (blue) galaxies** to **passive (red) galaxies** → did we find two modes of quenching?



SDSS-IV supported by Alfred P. Sloan foundation, U.S. Dept of Energy Office of Science and the Participating Institutions: sdss4.org

Next: study astrophysical trends



Isabella Olin
(U. Arizona, NOIRLab)

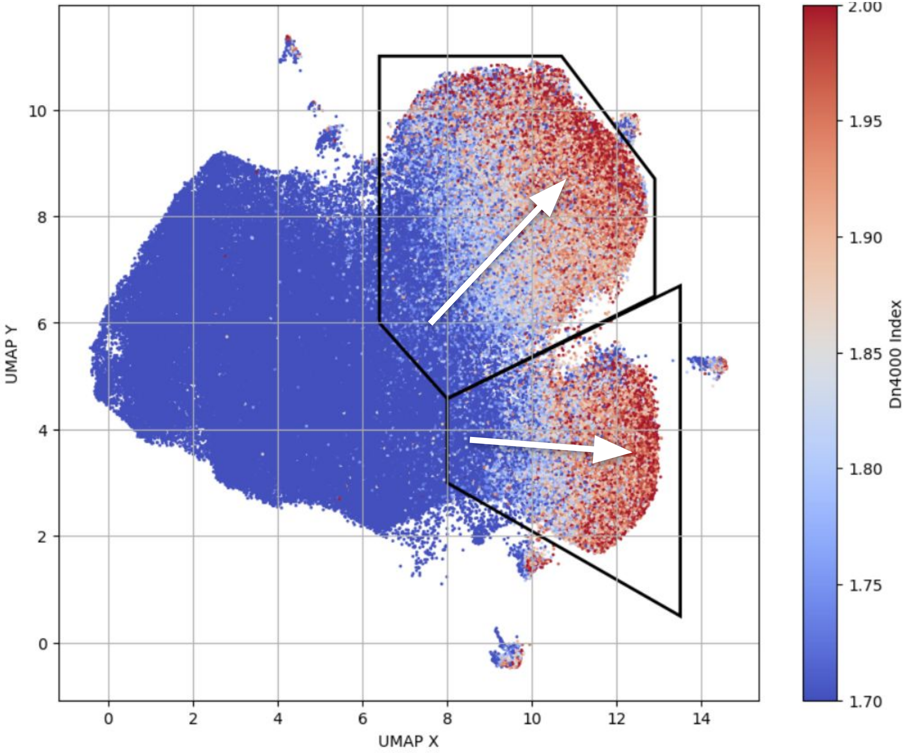
Revisit the UMAP projection and investigate astrophysical properties

Expect that passive galaxies have older stellar populations
⟶ stronger 4000-Angstrom break
⟶ red colors (r-z)

(Olin, SJ et al.; in prep.)

Expected: Gradient in stellar age

Age proxy = 4000-Angstrom Break (D_n4000)



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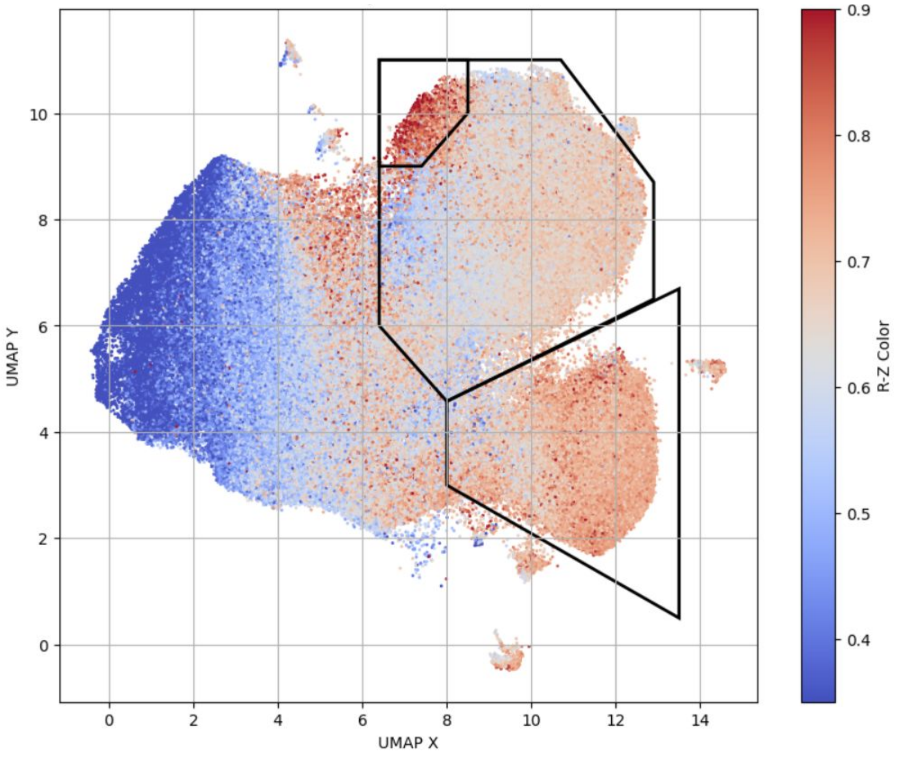
(Olin, SJ et al.; in prep.)

Unexpected: red outliers!

Optical (r-z) color



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Found outlier region of extremely red colors

Build a control sample matched in stellar mass and 4000-A break values and compare average spectra:

(Olin, SJ et al.; in prep.)

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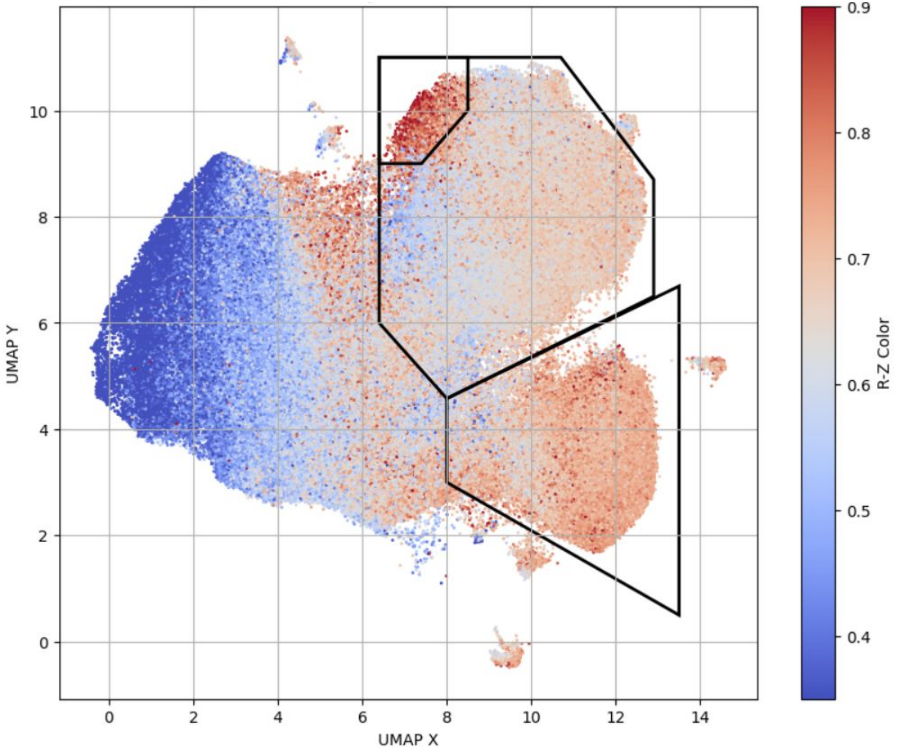


Found outlier region of extremely red colors

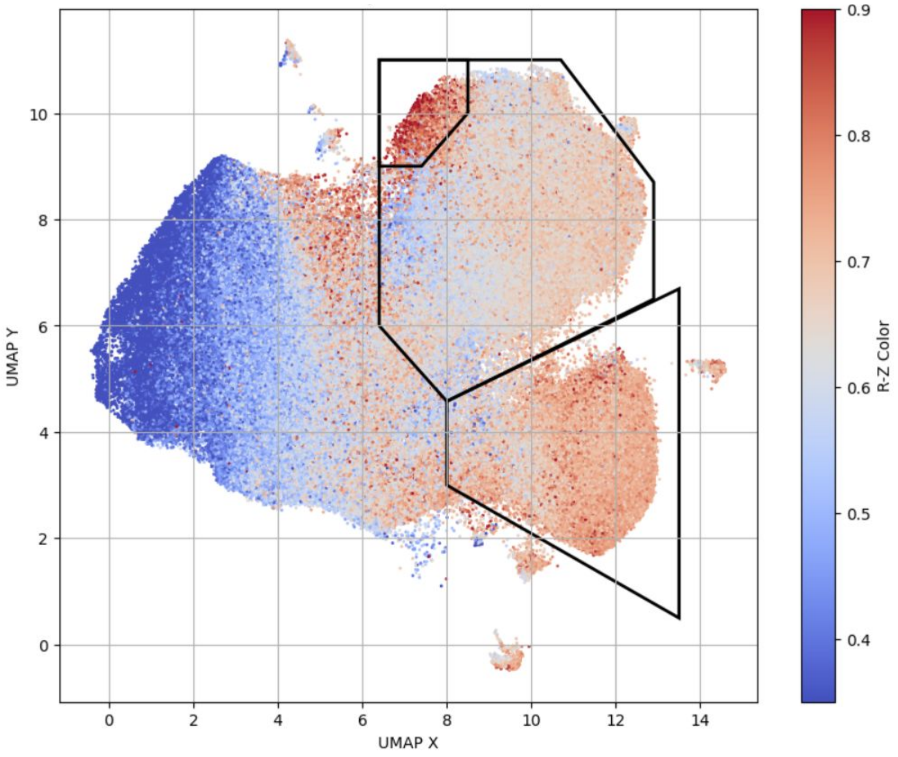
Build a control sample matched in stellar mass and 4000-A break values and compare average spectra:

- Outlier spectrum: best fit with significant dust reddening
- Control spectrum: best fit with nearly no dust reddening

(Olin, SJ et al.; in prep.)

Unexpected: red outliers!

Optical (r-z) color



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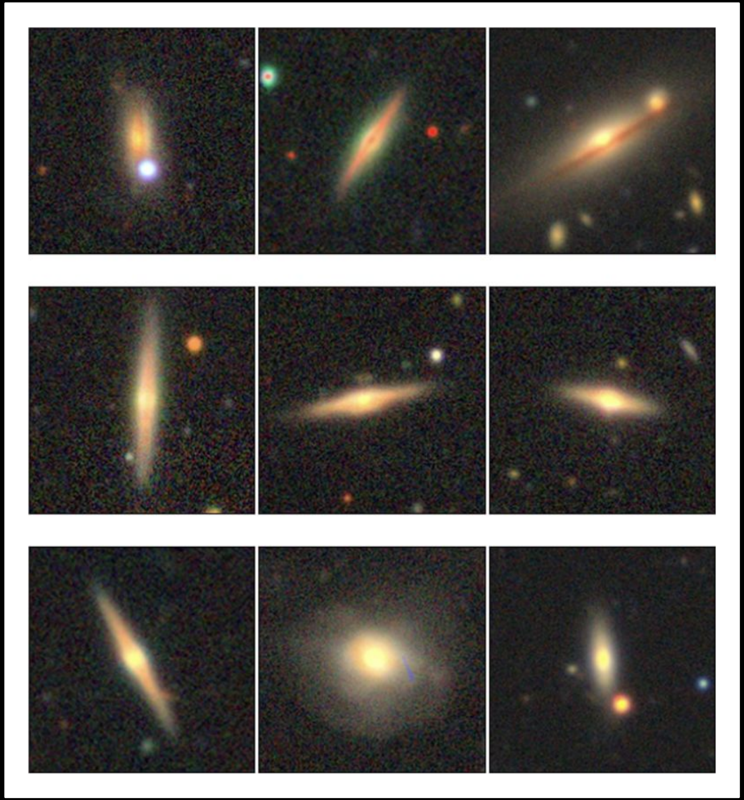
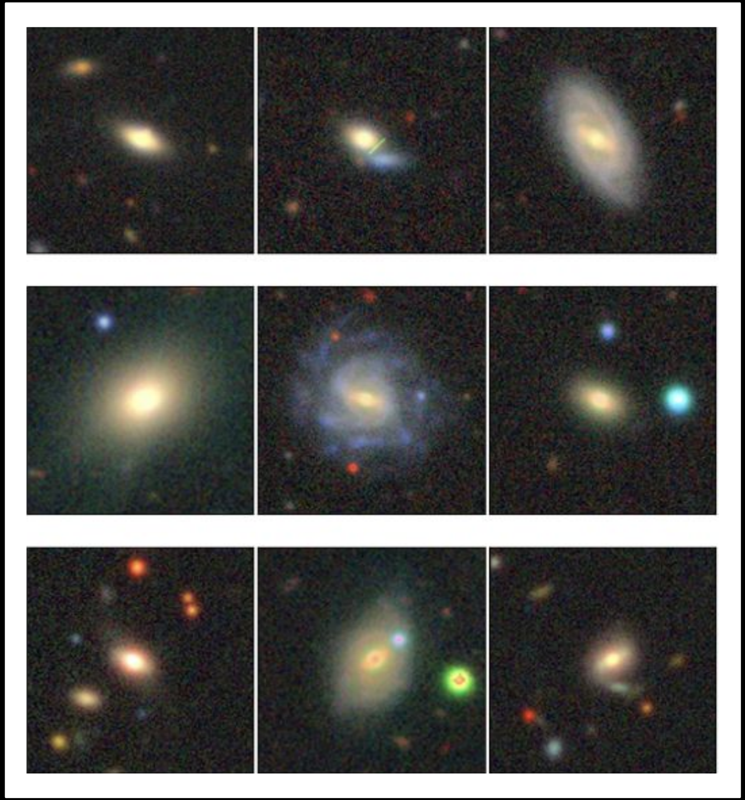
→ Check images for more clues

Outlier Galaxies



Control Galaxies

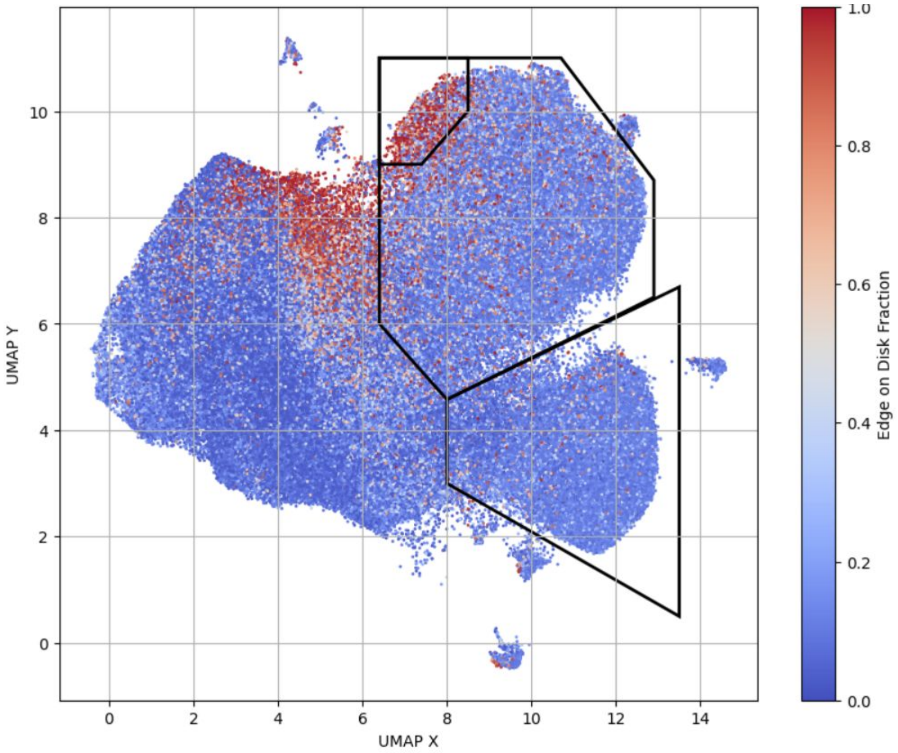


(**Olin**, Juneau et al., in preparation)

Legacy Survey DR9 (LS Viewer)

Unexpected: red outliers!

Edge-On Disk (class fraction)



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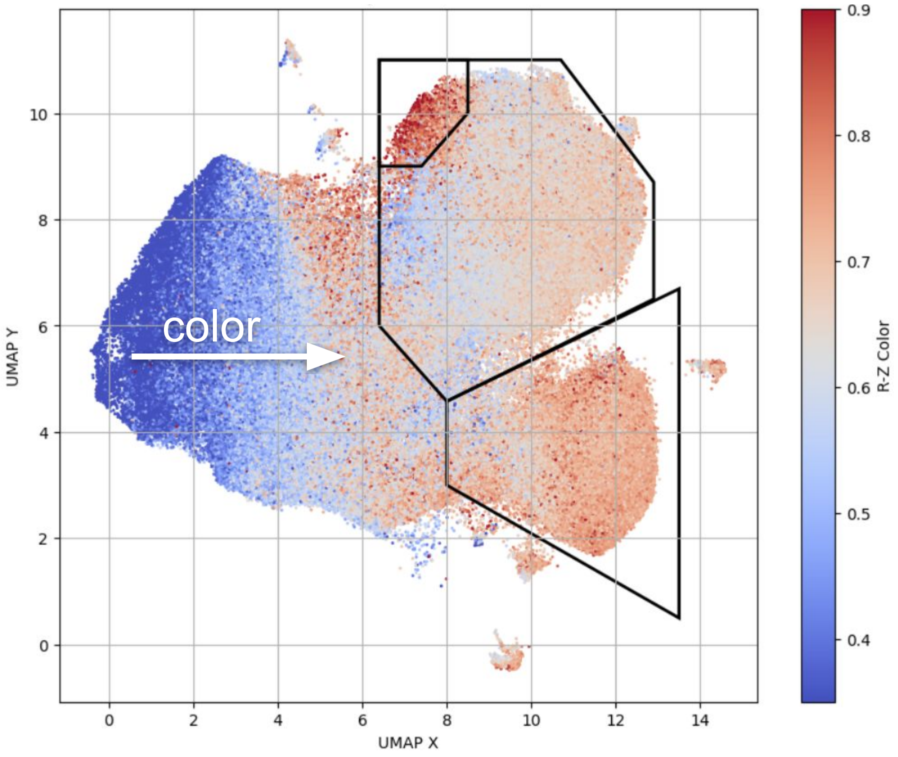
(U. Arizona, NOIRLab)

→ Confirm trend with edge-on disk based on ZooBot catalog (Walmsley+23), an ML algorithm trained on Galaxy Zoo visual classifications by citizen scientists

Star-forming galaxies show color gradient

Optical (r-z) color



Isabella Olin
(U. Arizona, NOIRLab)

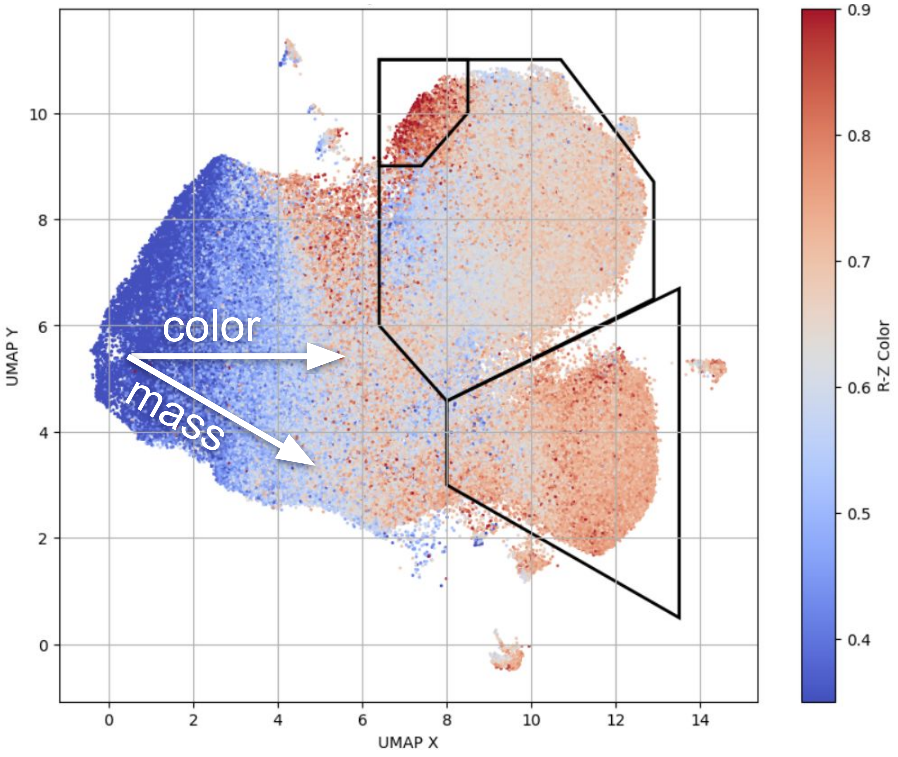
What about the star-forming galaxies?

→ astrophysical trend(s) along one axis from blue to red galaxies
(more to less star formation and/or less to more dust)

***note**: cannot directly interpret distances and directions in PAE latent space

Star-forming galaxies show color gradient

Optical (r-z) color



Isabella Olin
(U. Arizona, NOIRLab)

What about the star-forming galaxies?

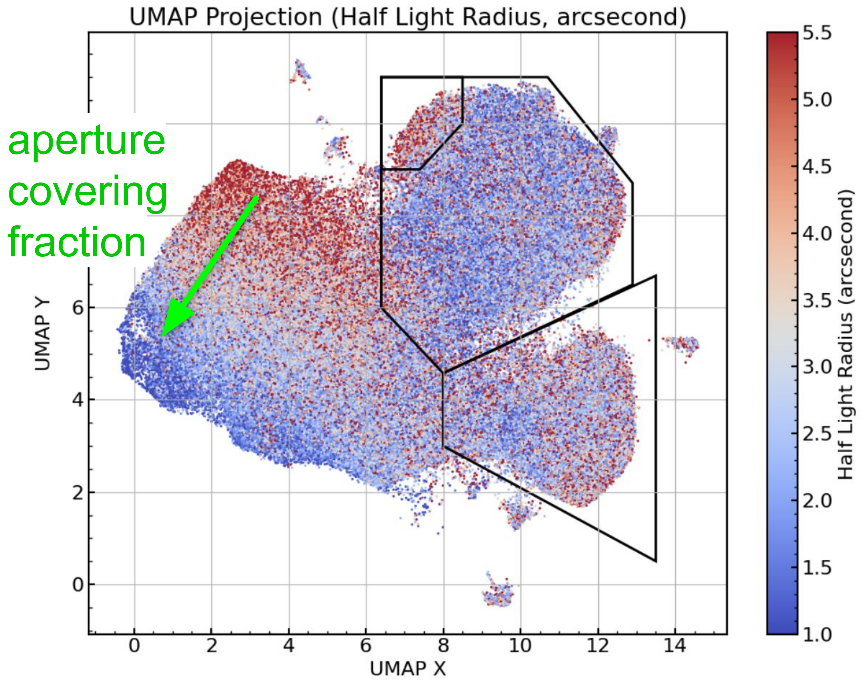
→ astrophysical trend(s) along one axis from blue to red galaxies
(more to less star formation and/or less to more dust)
→ stellar mass trend from low to high-mass

***note**: cannot directly interpret distances and directions in PAE latent space

Unexpected: trend with angular size?

Isabella Olin
(U. Arizona, NOIRLab)

Half-ligth angular size (arcsec)



<u>Notice trend on the star-forming side:</u>
large to small angular sizes ⟶ small to large aperture covering fraction

Unexpected: aperture covering fraction

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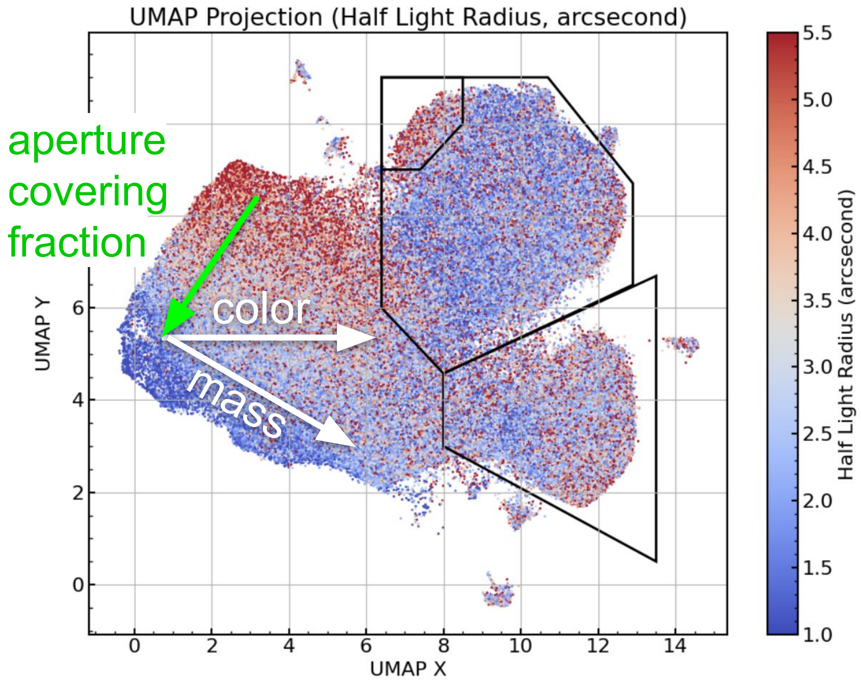
Half-ligth angular size (arcsec)



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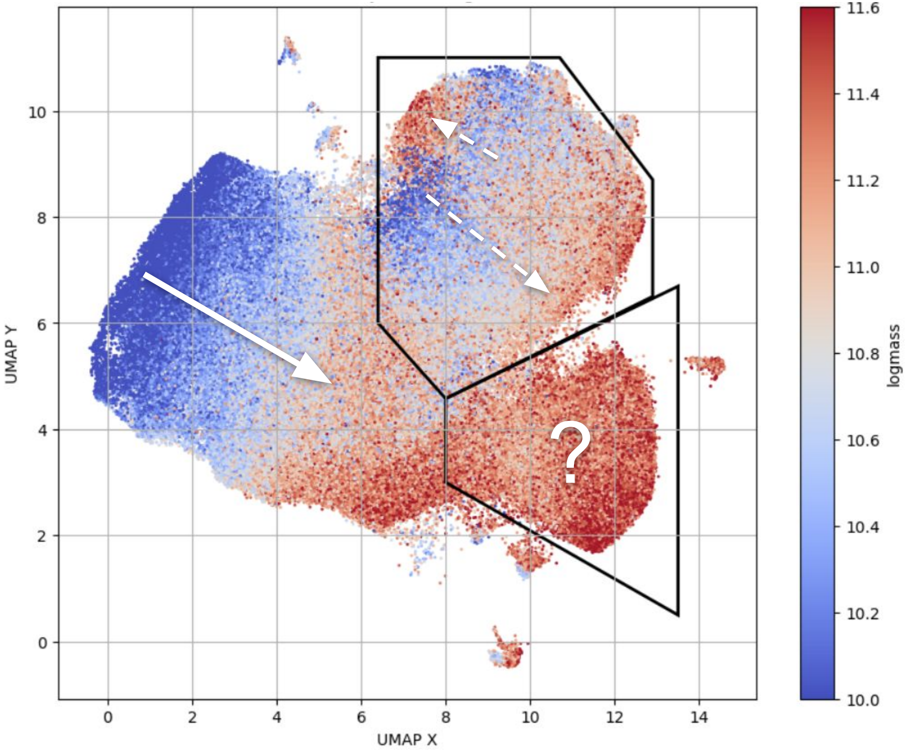
Nuanced trends with stellar mass

Log(Stellar Mass [$M_{\odot}$])



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Revisit the UMAP projection and investigate astrophysical properties

Expect that passive galaxies have older stellar populations
⟶ stronger 4000-Angstrom break
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⟶ **massive galaxies or quenched satellites**

(Olin, SJ et al.; in prep.)

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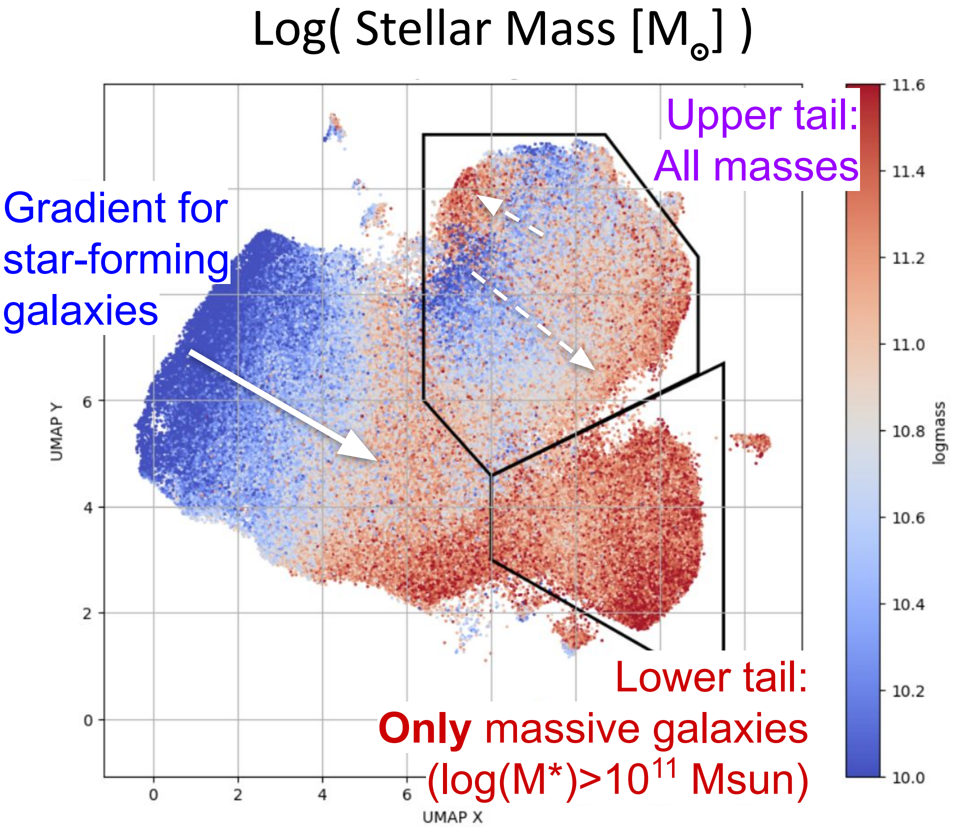

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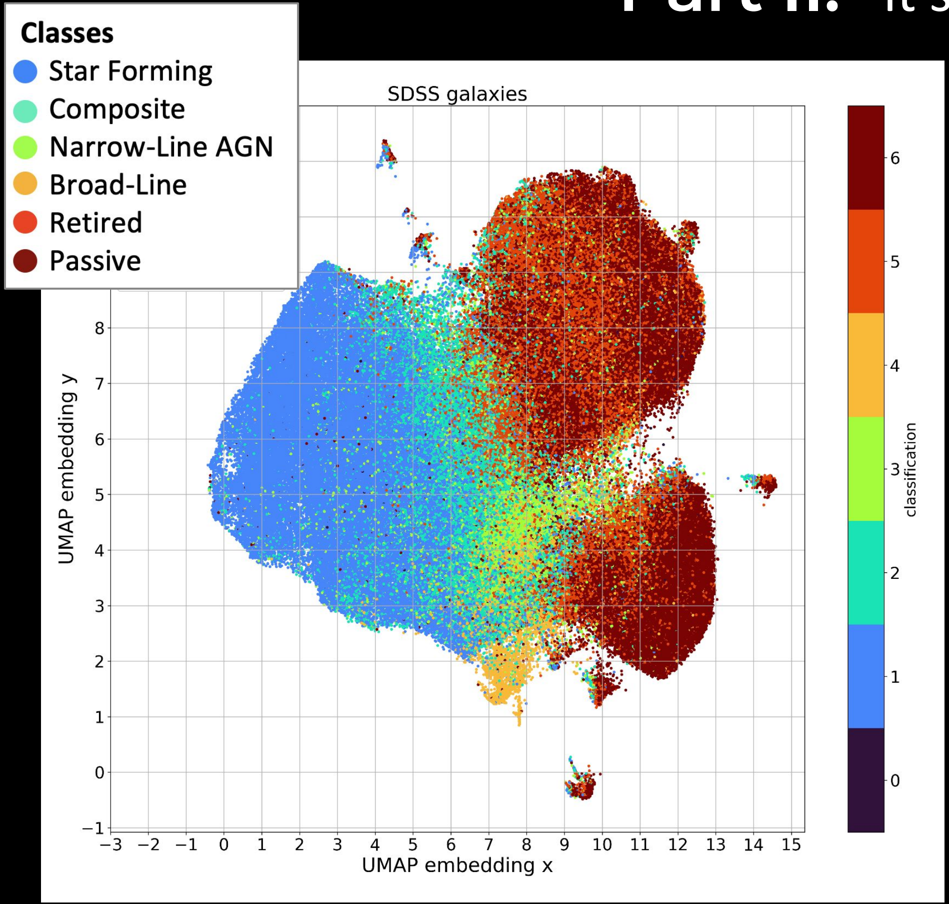
Part II: "it's complicated"

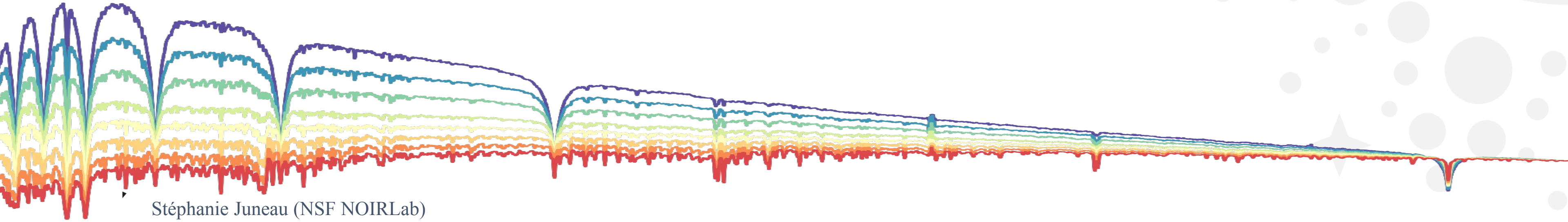


- Found signatures of old stellar ages supporting quenching (D_n4000, Hδ index)
- Two sequences (blobs) strongly differentiate in stellar mass and even more strongly in redshift → selection effects?
- AE+UMAP seem more sensitive to continuum shape than line features/indices
- AE+UMAP produce interesting outlier region of very dust-reddened edge-on galaxies (*without* morphological info)

(**Olin**, Juneau et al., in preparation)

Take away: Spectroscopy encodes it all

- Used dimensionality reduction (PAE + UMAP) on ~200,000 SDSS spectra and found that unsupervised model is learning *simultaneously*:
  - Astrophysical trends (galaxy star formation activity ⟶ from star-forming to passive)
  - Aspects normally associated with images (galaxy morphology / orientation)
  - Survey design/experimental set-up (aperture covering fraction)
  - Selection effects (survey detection limit – not shown)

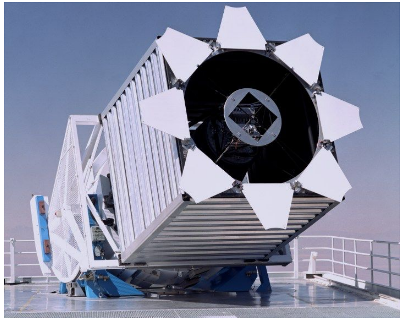


Stéphanie Juneau (NSF NOIRLab)

From SDSS to DESI

Sloan Digital Sky Survey (SDSS)

- SDSS I-IV: Long legacy of 25+ years
- DR17 includes **5.8 Million spectra** of stars, galaxies & quasars (SDSS+BOSS)



SDSS-IV supported by Alfred P. Sloan foundation, U.S. Dept of Energy Office of Science and the Participating Institutions: sdss4.org

Dark Energy Spectroscopic Instrument (DESI) on Kitt Peak, AZ

- Will obtain spectra of **63 M galaxies and quasars** in 2021-2029
- DR1 already the largest sample of (~20 Million) optical spectra of stars, galaxies, quasars
- Cosmology results: hints for evolving Dark Energy but still consistent with LCDM

DESI Collaboration/KPNO/NOIRLab/NSF/AURA/P. Horálek/R. Proctor

DESI is funded by the U.S. Department of Energy Office of Science: data.desi.lbl.gov/doc/acknowledgments

ML/AI models of spectra

How can we harness ML/AI while not misinterpreting our findings (selection effects *vs.* astrophysics)?

Follow-up work

Repeat a new experiment with DESI [larger sample size, different selection effects (Andy Morgan's talk)] with a multi-modal approach [e.g., AstroCLIP (Parks+24), AstroPT (Smith+24), AVIS (Yufeng Luo's talk)]

Credit: D. Schlegel/Berkeley Lab using data from DESI

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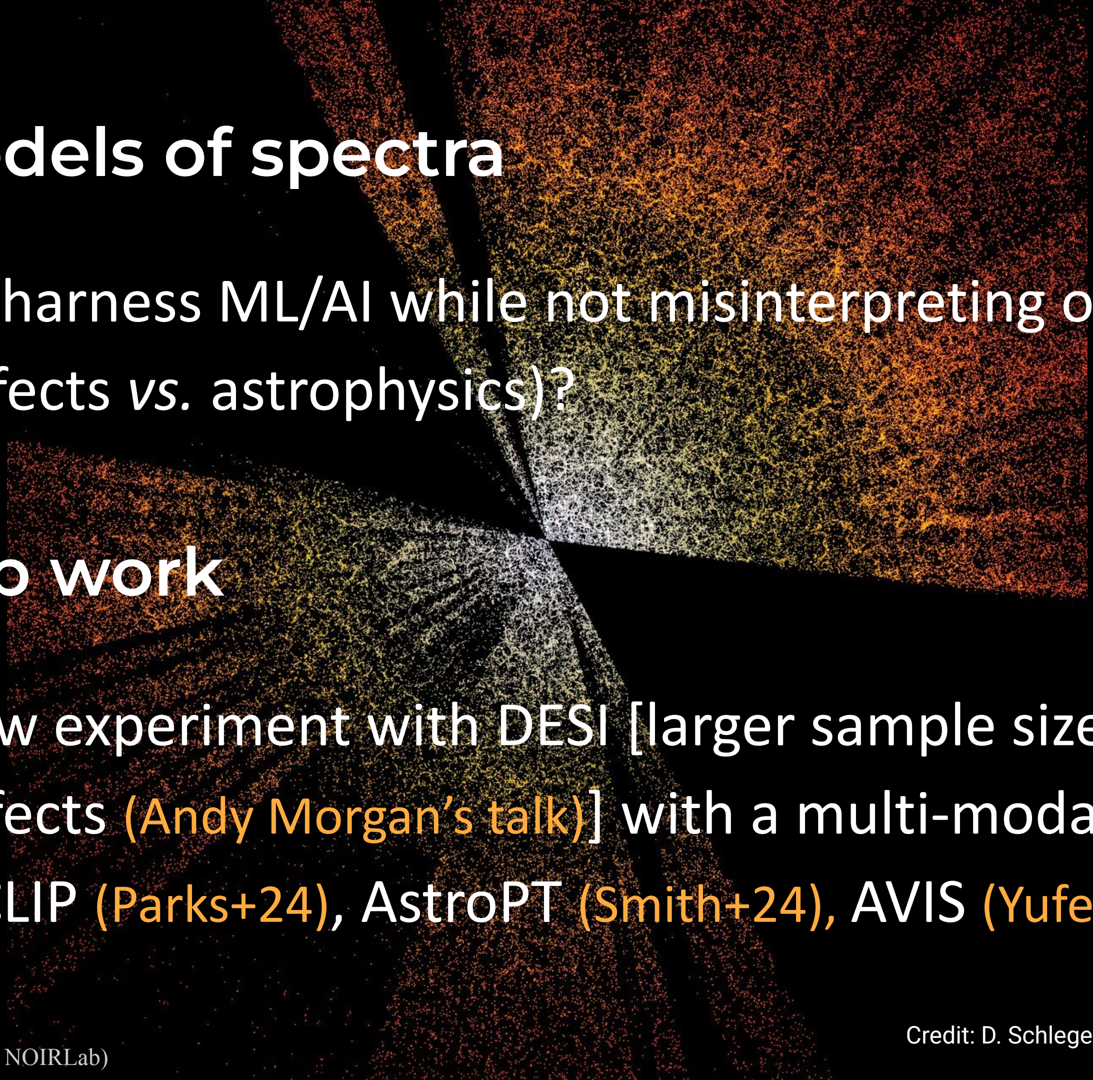
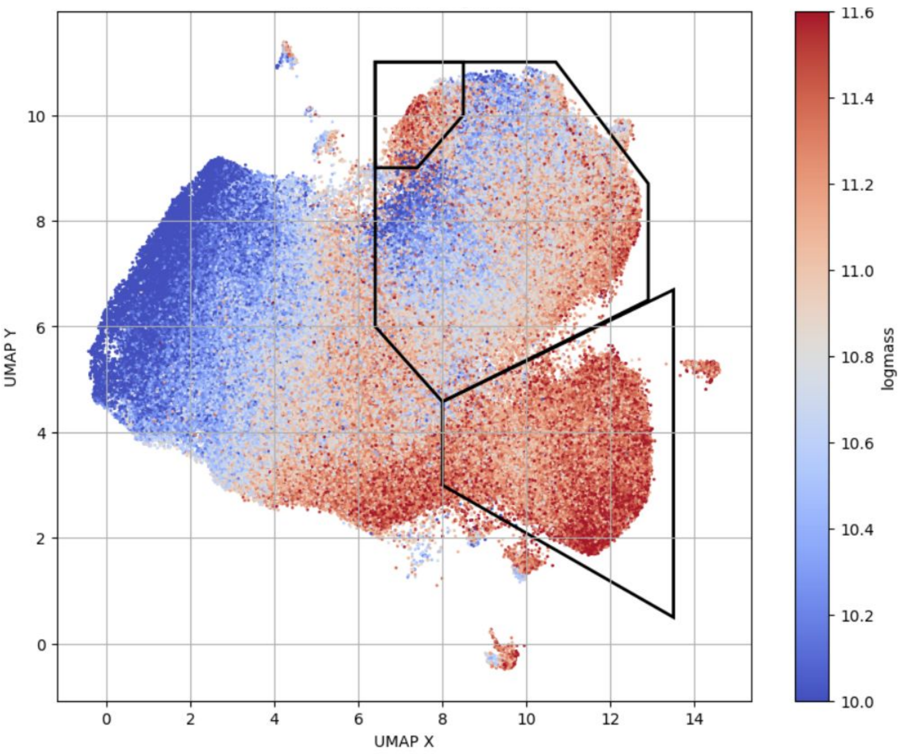


Credit: D. Schlegel/Berkeley Lab using data from DESI

Thank you!

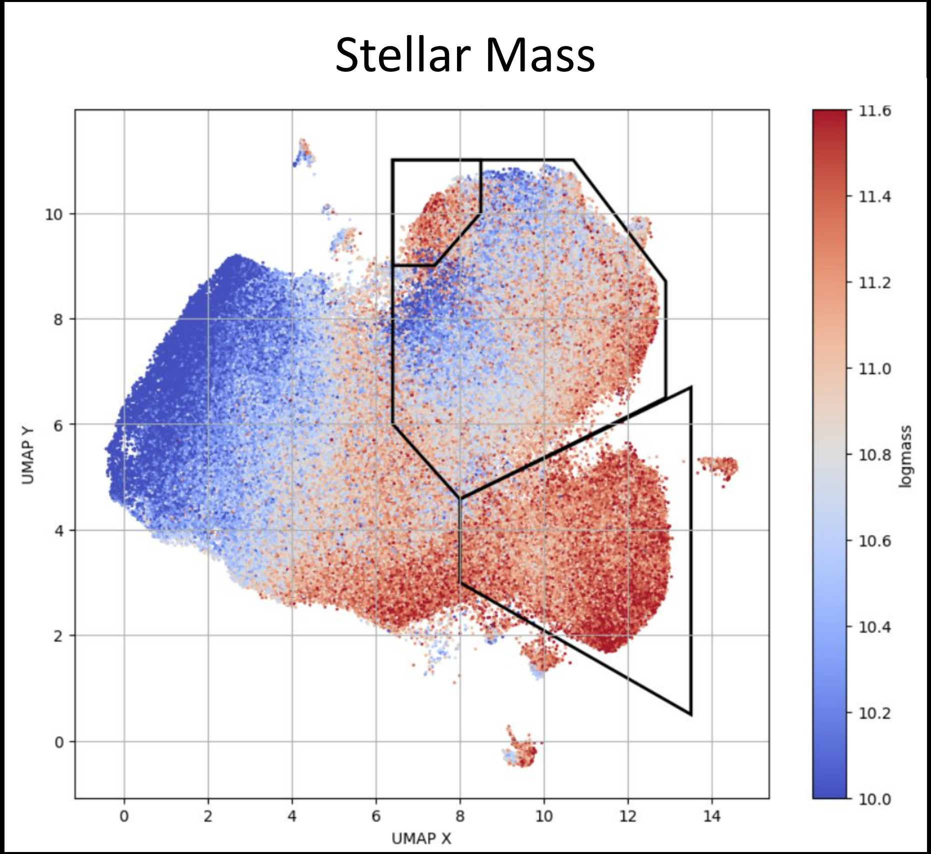
ESA/Hubble & NASA

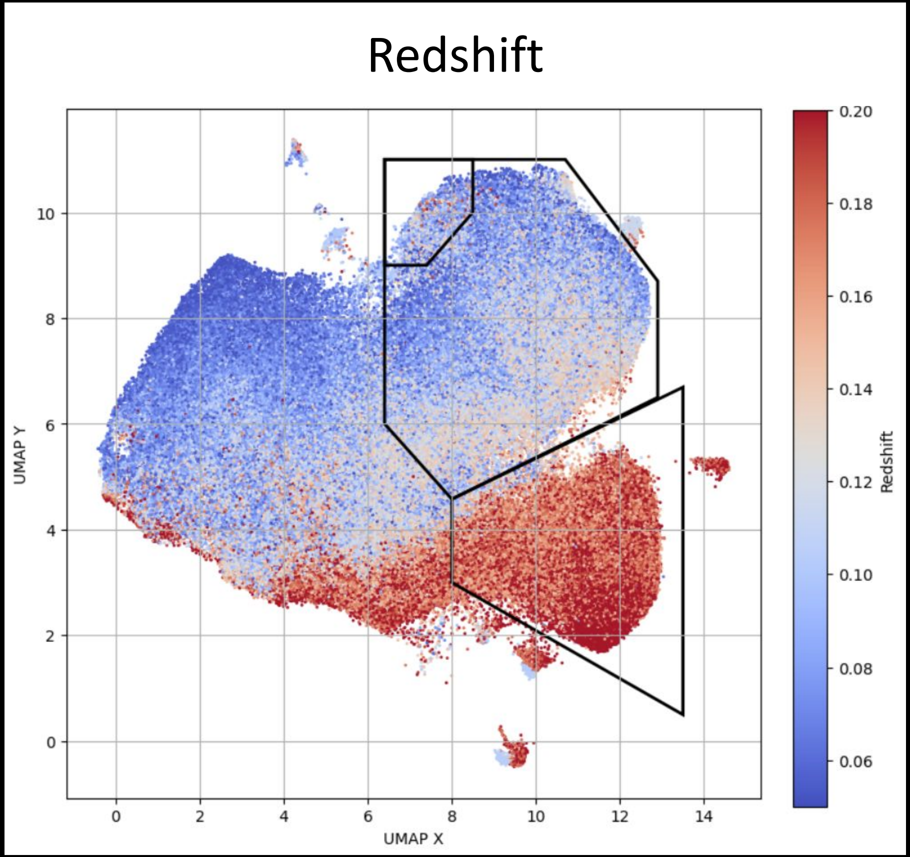
Stellar Mass



(**Olin**, Juneau et al., in preparation)

!! Need to consider selection effects !!





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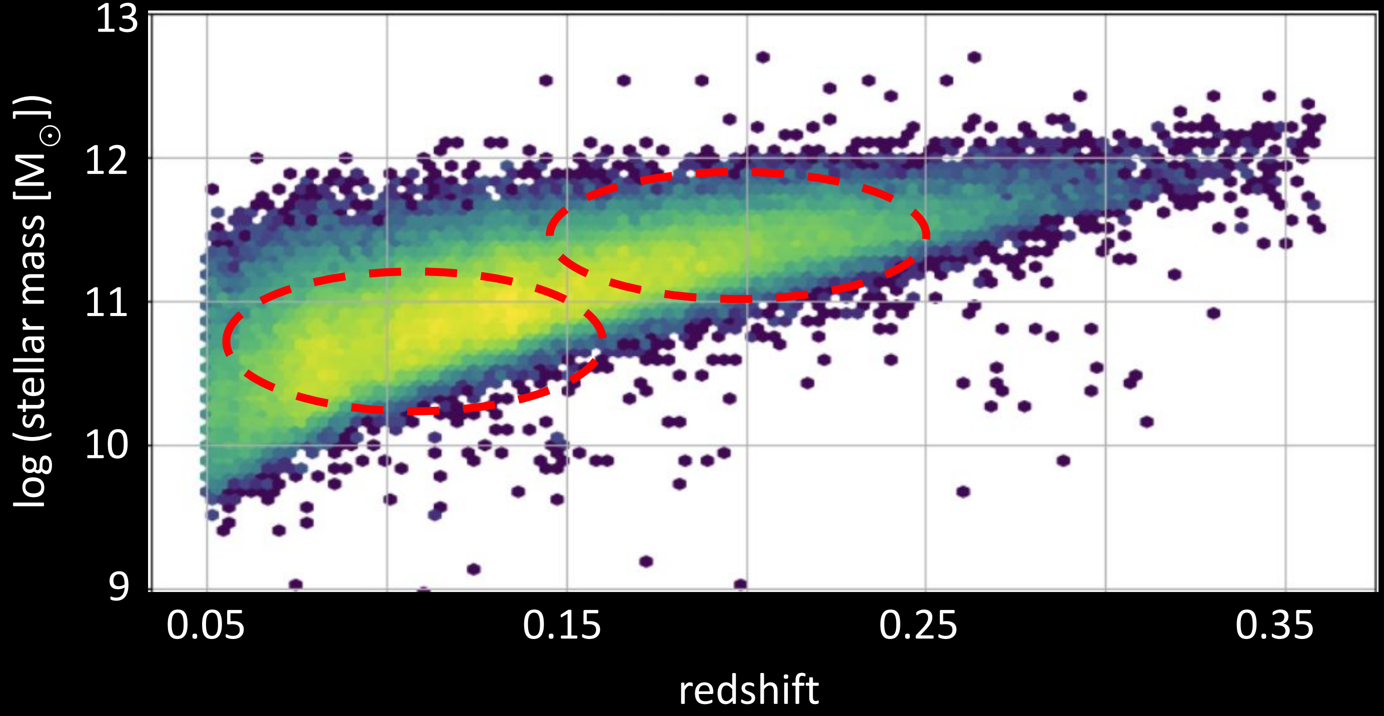
Stellar mass vs. redshift



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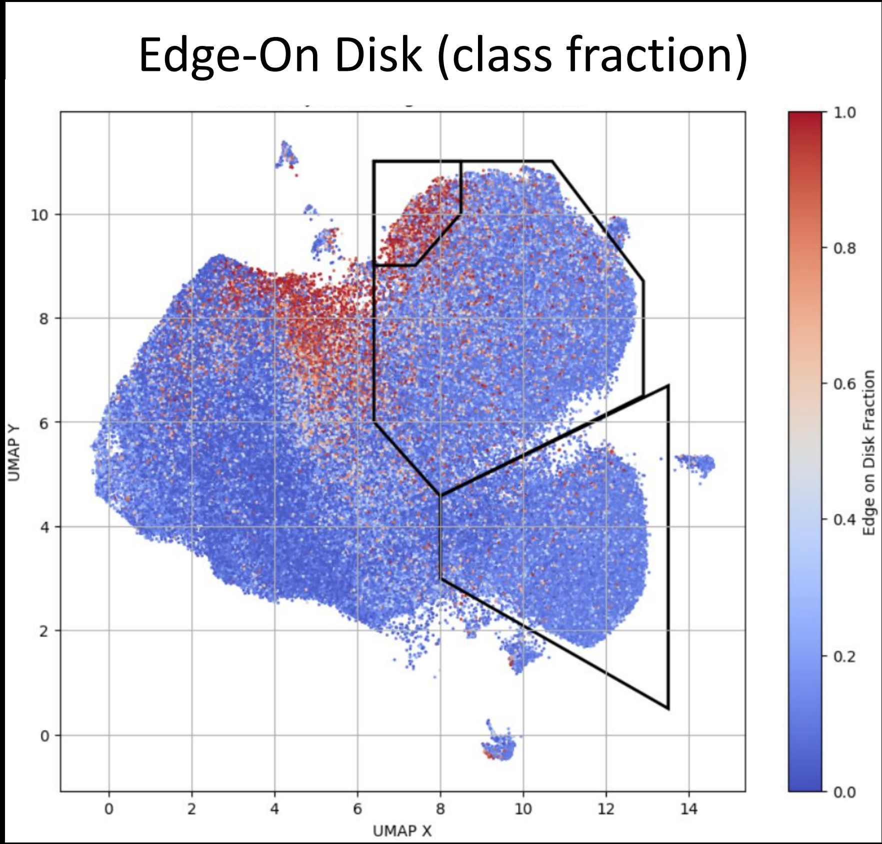
Generalizing with Zoobot (Bot trained on Galaxy Zoo)

Galaxy Zoo is based on visual classification by citizen scientists (Lintott+2008)

Recent work to automate classification with ML applied to DESI Legacy Survey images (Walmsley+2023)

Train model to predict visual classifications for certain features.

Fraction of scientists who would answer "yes" to Is there an EDGE-ON DISK?



(**Olin**, Juneau et al., in preparation)

SDSS DR16 Galaxy sample

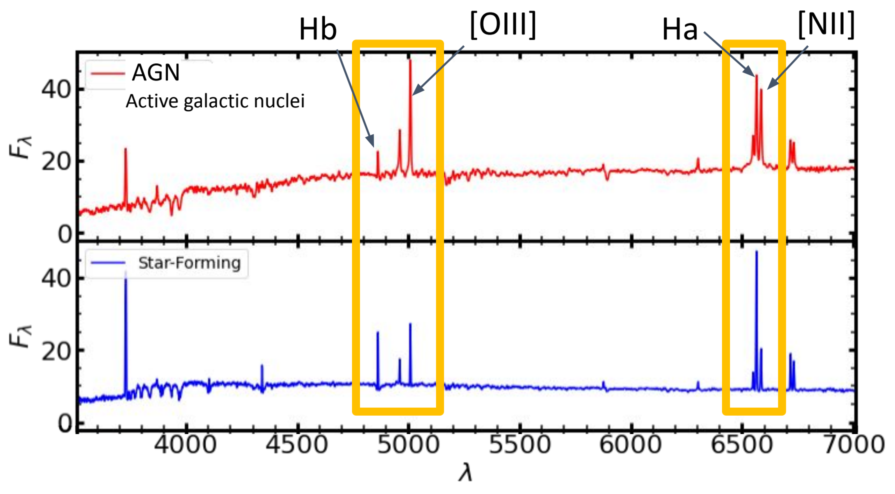
(SDSS = Sloan Digital Sky Survey)

Classes
- Star Forming
- Composite
- Narrow-Line AGN
- Broad-Line
- Retired
- Passive

- Sample: 210,000 (training) and 140,000 (test)
- Low redshift galaxies (0.05 < z < 0.36)
- Create labels with traditional emission-line diagnostic diagrams

CLASS = GALAXY or QSO
PLATEQUALITY = “good”
ZWARNING = 0
0.05 < z < 0.36
Masked fraction < 40% of pixels
Cumulative S/N>50
Rebin to N=1000 elements

⟶ training set: 209,462
⟶ test set: 139,642



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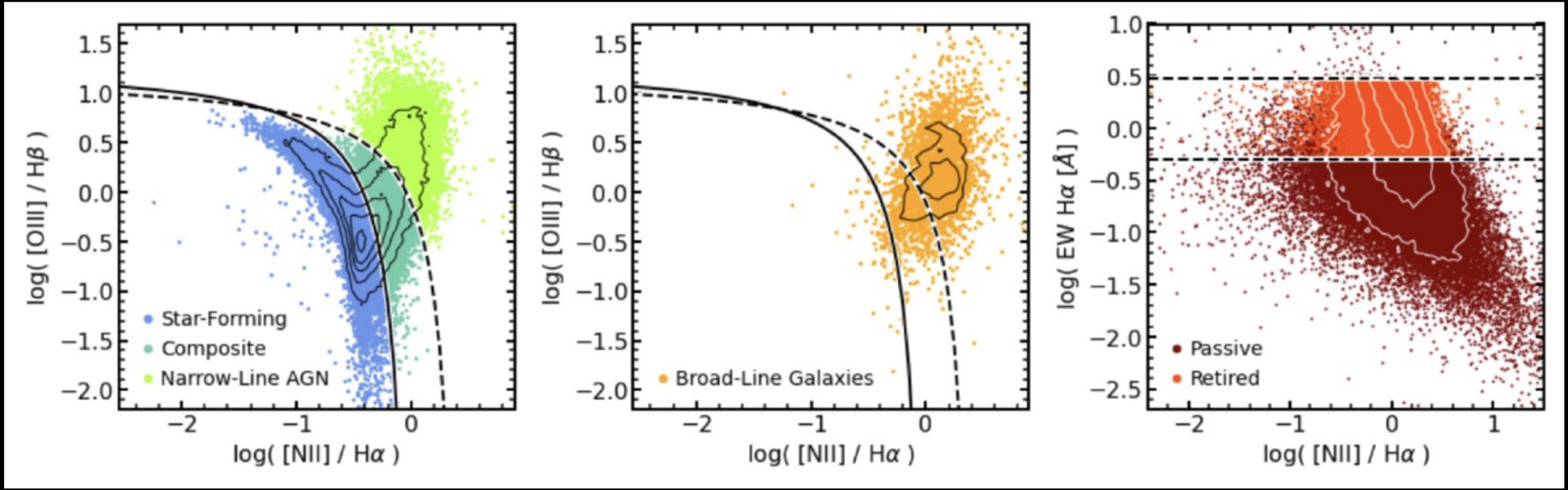
Classification combining BPT & WHAN diagrams



Classes
- Star Forming
- Composite
- Narrow-Line AGN
- Broad-Line
- Retired
- Passive

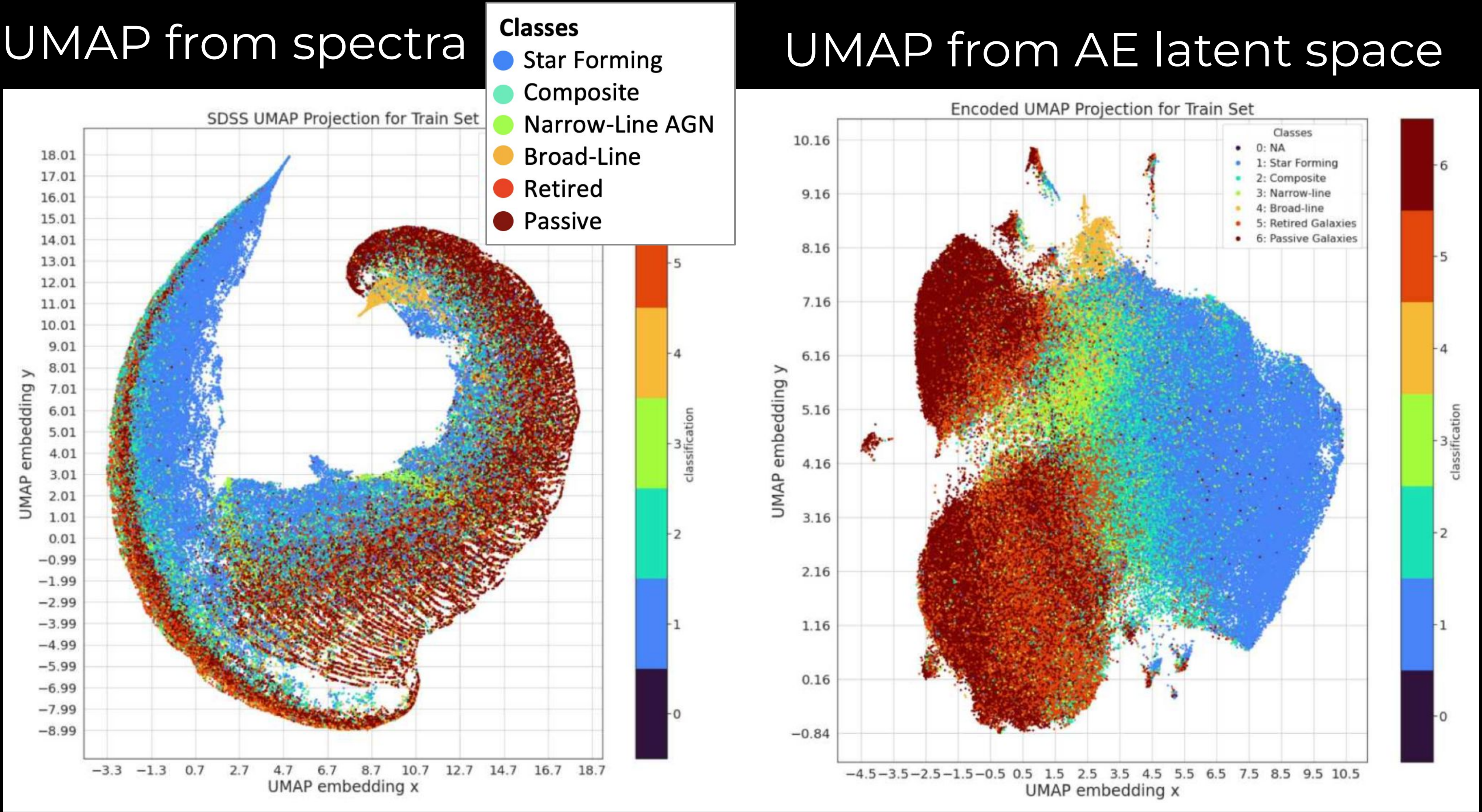
(Left) Star-Forming, Composite and Narrow-line AGN **(Middle)** BROADLINE flag is set in SDSS ⟶ Broad-line AGN; **(Right)** Retired & Passive galaxies

WHAN: Equivalent width of Halpha vs. [NII]/Ha ratio (Cid-Fernandes et al. 2011)

(Pat, Juneau, Böhm et al.; arXiv:2211.11783)

UMAP from spectra

UMAP from AE latent space

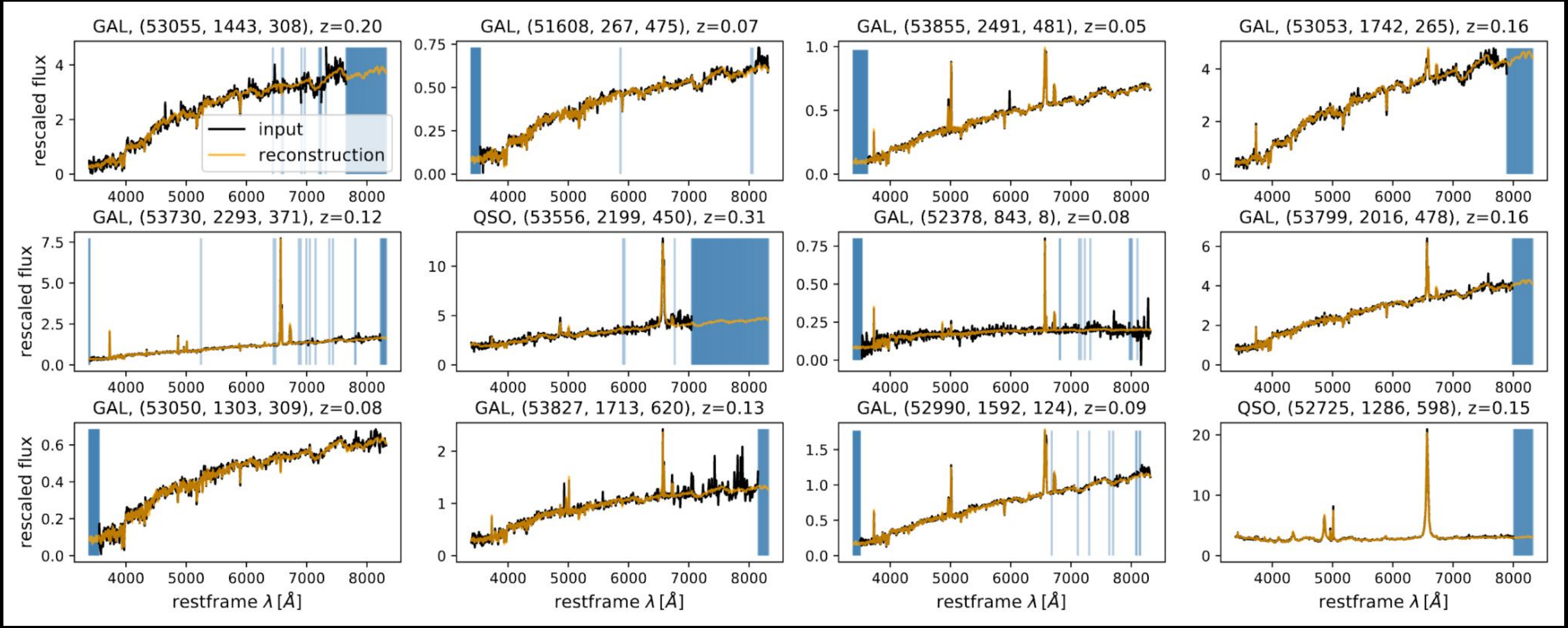


(Pat, Juneau, Böhm et al., 2022)

Example PAE-reconstructed SDSS spectra

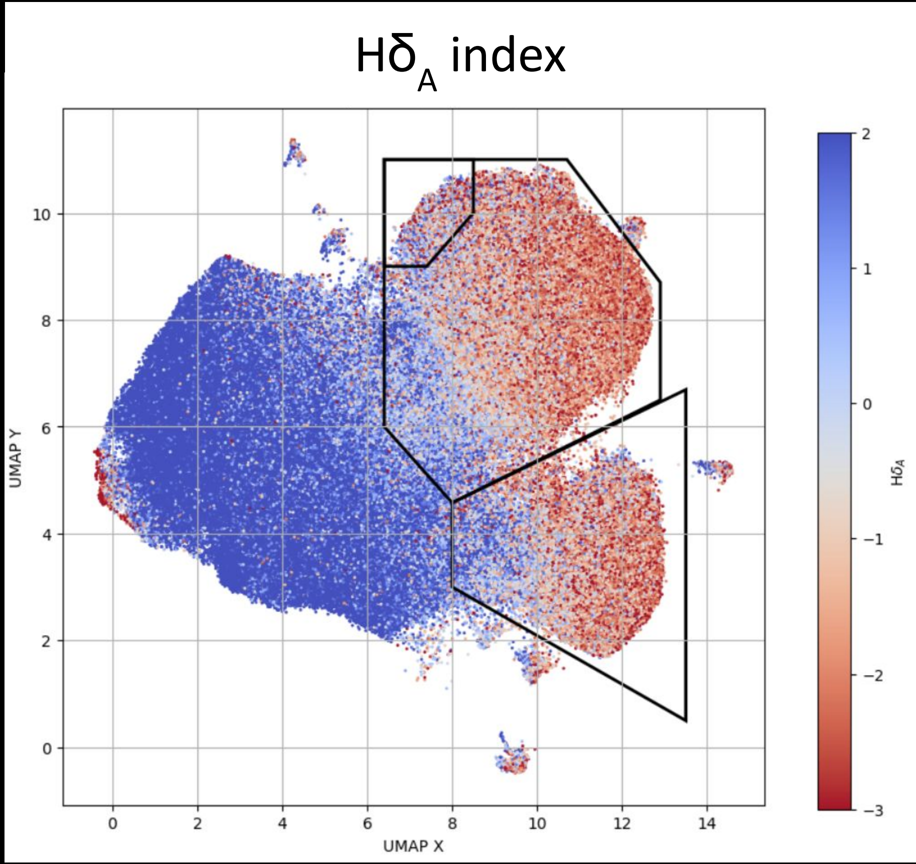
Black: observed spectra (noisy with masked regions)
Orange: denoised and inpainted reconstructed spectra

CLASS (MJD, PLATE, FIBERID)



(Böhm, Kim & Juneau 2023)

Isabella Olin
(U. Arizona, NOIRLab)



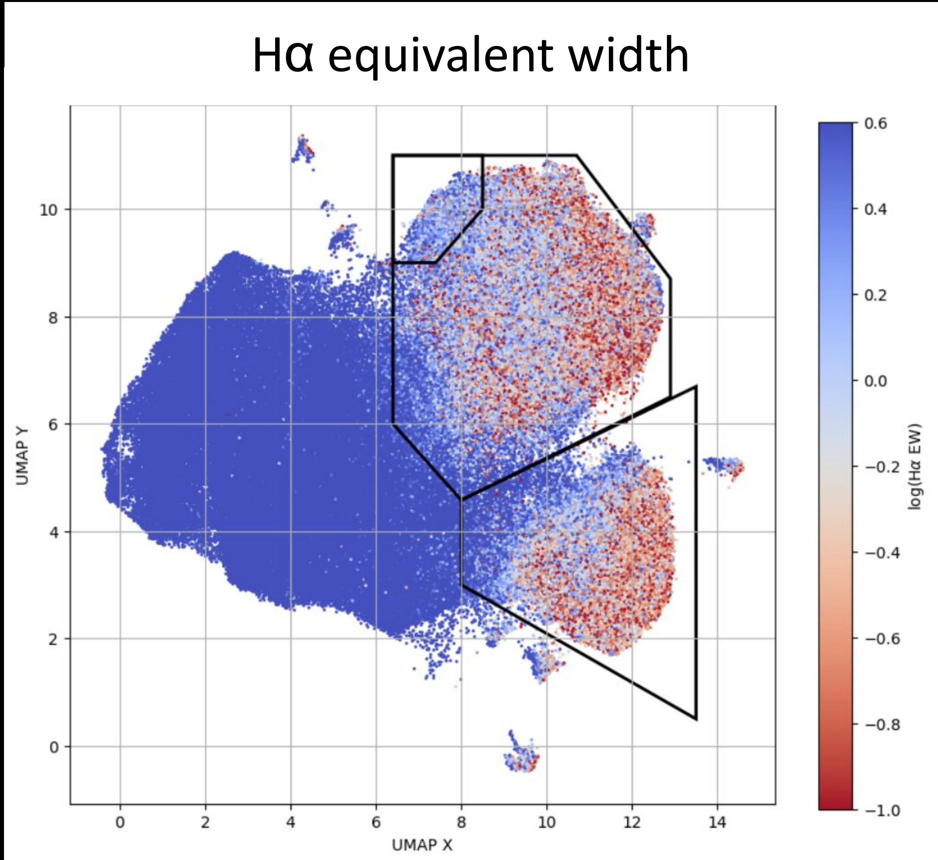
(**Olin**, Juneau et al., in preparation)

Revisit the UMAP projection and investigate astrophysical properties

Expect that passive galaxies have older stellar populations
→ stronger 4000-Angstrom break (D_n4000)
→ weaker H-δ index

<u>Next:</u>
Expect passive galaxies to be either massive centrals (easy to detect) or satellites (missing from samples)

Isabella Olin
(U. Arizona, NOIRLab)



(**Olin**, Juneau et al., in preparation)

Revisit the UMAP projection and investigate astrophysical properties

Expect that passive galaxies have older stellar populations
→ stronger 4000-Angstrom break (Dn4000)
→ weaker H-δ index

And less star formation
→ weaker H-alpha EW

Next: Expect passive galaxies to be either massive centrals (easy to detect) or satellites (missing from samples)

DESI Data Access

DESI: data.desi.lbl.gov

Acknowledgments: data.desi.lbl.gov/doc/acknowledgments/

DESI Collaboration et al. 2024b (arXiv:2306.06308)

Astro Data Lab: datalab.noirlab.edu

Acknowledgments: datalab.noirlab.edu/acknowledgments.php

Nikutta et al. 2020, AsCom 33, 100411; Fitzpatrick et al. 2014, SPIE 9149

SPARCL: astrosparcl.datalab.noirlab.edu

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