



Supervised deep learning methods for Rubin LSST Image classification, mass modeling, and photometric redshift prediction

Raoul Cañameras (MPA/TUM → LAM after 1.12.2023)

rcanameras@mpa-garching.mpg.de

Seminaire pole ML/DL du CeSAM

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Strong gravitational lensing





Massive galaxy or galaxy cluster bends space-time

Strong lensing regime: Elongated arcs + multiple images of the background galaxy

Strong gravitational lensing

1 - Static background sources, e.g. distant galaxies



Studies of galaxy evolution and dark-matter distribution:

- Total mass of the foreground lens galaxy/cluster
- High-resolution studies of magnified background galaxies

Strong gravitational lensing

2 – Time-variable sources, e.g. quasars, supernovae



Searching for new strong gravitational lenses Case of static galaxy-galaxy lensing systems

Simple binary classification problem (lens vs nonlens) BUT

Strong lensing events are very rare \rightarrow 1 galaxy out of 10⁴ or 10⁵ in a given data set

Need to exclude a wide range of contaminants: Spirals, ring galaxies, mergers, etc...

Need to get rid of image artefacts automatically + Ensure position/rotation invariance



Fig. Examples of strong lens candidates from DECaLS

Various types of nonlens contaminants (from Huang et al. 2021)

Searching for new strong gravitational lenses Case of single or multi-band imaging data sets



Rubin LSST 10⁵ new lenses (Collett 2015)

Supervised Deep Learning classification

e.g. in CFHTLS (Jacobs+2017); COSMOS HST (Pourrahmani+2018); KiDS (e.g., Petrillo+2017; +2019; Li+2020, Li+2021); DES (e.g., Jacobs+2019a,b, Rojas+2022); DECaLS (e.g., Huang+2020; +2021, Storfer+2022); CFIS (e.g., Savary+2022); DELVE (e.g., Zaborowski+2023)

systematically outperforms non-ML algos

e.g. Arc-finder algorithms (e.g., Gavazzi+2014, Avestruz+2019); Principal component analyses (e.g., Joseph+2014; Paraficz+2016); Lens modeling and masking (e.g., Sonnenfeld+2018); Citizen-science projects (e.g., Marshall+2016, Sonnenfeld+2020); Visual inspection (e.g., Diehl+2017, Khullar+2021)



YATTALENS arcfinder applied to HSC (Sonnenfeld+2018)

Name	Туре	AUROC	TPR_0	TPR_{10}	Short description		
CMU-DeepLens-Resnet-ground3	Ground-based	0.98	0.09	0.45	CNN		
CMU-DeepLens-Resnet-Voting	Ground-based	0.98	0.02	0.10	CNN		
LASTRO EPFL	Ground-based	0.97	0.07	0.11	CNN		
CAS Swinburne Melb	Ground-based	0.96	0.02	0.08	CNN		
AstrOmatic	Ground-based	0.96	0.00	0.01	CNN		
Manchester SVM	Ground-based	0.93	0.22	0.35	SVM/Gabor		
Manchester2	Ground-based	0.89	0.00	0.01	Human Inspection		
ALL-star	Ground-based	0.84	0.01	0.02	Edges/gradiants and Logistic Reg.		
CAST	Ground-based	0.83	0.00	0.00	CNN/SVM		
YattaLensLite	Ground-based	0.82	0.00	0.00	SExtractor		

 Table. Results of lens-finding challenge (Metcalf+2019)

Supervised machine learning classification



Neural Networks



Fig. Credit Leal-Taixe, Niessner

Convolutional Neural Networks

CNNs are supervised machine learning techniques optimized for image analysis (LeCun+1998) Capture image characteristics by learning the coefficients of convolutional kernels Need at least 10⁴ labelled images for training BUT only ~10³ lenses known



Automated pipelines for wide-field imaging surveys

Several hundred candidates from CNNs in the literature

Elevated confirmation rate >80% (Tran et al. 2022)

BUT drastic pre-selection to cope with data volumes

We need fully automated, all-sky searches for current surveys and for Rubin LSST

+ Extend deep learning methods to mass modeling and photometric redshift estimation



Fig. Follow-up of AGEL lenses (Tran+2022)



Projects part of HOLISMOKES (Suyu+2020)

(Highly Optimized Lensing Investigations of Supernovae, Microlensing Objects, and Kinematics of Ellipticals and Spirals)







Cañameras et al. 2020, A&A 644, 163

Systematic strong-lens search over the Pan-STARRS 3π survey (30 000 deg²)

→ $3x10^9$ sources to be classified

Realistic lens simulations for high classification accuracies

Need realistic lens galaxies, good proxies of lens mass, Einstein radius distributions, number of multiple images, source colors and morphologies

+ match properties of PanSTARRS coadds (sky background, inclusion of neighbours and artifacts, good PSF models, etc)

- → Paint lensed arcs on survey stacks
- → 10⁵ labelled examples





Cañameras et al. 2020, A&A 644, 163

Systematic strong-lens search over the Pan-STARRS 3π survey (30 000 deg²)

- → $3x10^9$ sources to be classified
- → 2.3×10^7 after simple photometric cuts, star removal

Two-step approach to cope with huge data volume

→ 1.0×10^6 after apply neural network on photometry



19 i_{R3}

Blue arcs

-0.55



Cañameras et al. 2020, A&A 644, 163

Systematic strong-lens search over the Pan-STARRS 3π survey (30 000 deg²)

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Two-step approach to cope with huge data volume

- → 1.0×10^6 after apply neural network on photometry
- → 1.2x10⁴ after apply convolutional neural network on g, r, i-band image cutouts







Cañameras et al. 2020, A&A 644, 163; Cañameras et al. 2021, A&A 6, L6



330 new high-quality lens candidates from Pan-STARRS, follow-up on-going (Taubenberger et al., in prep.)

Also successful on ~4 mag deeper imaging from HSC Wide survey (Cañameras et al. 2021, Shu et al. 2022)

Method for all-sky classification works + Applicable to the future Rubin LSST stacks



Lens candidates from HSC (Shu et al. 2022)



Cañameras et al. 2020, A&A 644, 163; Cañameras et al. 2021, A&A 6, L6



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Method for all-sky classification works + **Applicable to the future Rubin LSST stacks**

Not fully automated due to number of contaminants

Inspection of few 10⁴ to 10⁶ cutouts depending on survey depth



After few hours of "expert" visual inspection of lens candidates

BUT ALSO several false positives!

1.000



1.000

1.000

Cañameras et al. 2020, A&A 644, 163; Cañameras et al. 2021, A&A 6, L6





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Not fully automated due to number of contaminants

Inspection of few 10^4 to 10^6 cutouts depending on survey depth \rightarrow **Strong biases?**



Grading and regrading (Shu et al. 2022)

How can we reduce human input?

Cañameras et al. 2023, arXiv:2306.03136

- → Build test set from real survey data (e.g. HSC Wide)
 - 220 known galaxy-scale lenses (SuGOHI project)
 - → Test completeness for different configurations
 - 70,000 non-lenses in COSMOS
 - → Measure correct number of false positives

Metrics
→ area under ROC
→ TPR₀ and TPR₁₀

$$TPR = \frac{TP}{TP + FN}; FPR = \frac{FP}{FP + TN}$$







Cañameras et al. 2023, arXiv:2306.03136

The design of the ground-truth data set is key to improve performance

Interactive machine learning \rightarrow here by modifying the training sample iteratively

Test multiple **combinations of positive examples** (simulated lenses), fixing everything else

→ Balanced data sets of about 10⁵ examples



Cañameras et al. 2023, arXiv:2306.03136

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Parameter distributions chosen in simulations play a major role (no need to follow nature)



Cañameras et al. 2023, arXiv:2306.03136

The design of the ground-truth data set is key to improve performance

Interactive machine learning → here by modifying the training sample iteratively
 Test multiple combinations of negative examples (non-lenses), fixing everything else
 → Balanced data sets of about 10⁵ examples



Drawing random non-lenses does not work

→ Need to boost fractions of usual contaminants (spirals, rings, groups, etc)

→ Use external citizen science projects or unsupervised ML classifications



Our goal

Cañameras et al. 2023, arXiv:2306.03136

Fine-tuning the network architecture also plays a major role

Test multiple **network architectures**, fixing everything else



Cañameras et al. 2023, arXiv:2306.03136

The processing of the ground-truth data set is important

Test multiple data augmentation techniques, fixing everything else

→ Balanced data sets and baseline ResNet architecture



Evaluation of supervised neural networks - Summary

Cañameras et al. 2023, arXiv:2306.03136

- Major improvements for specific networks and data sets → FPRs from 1% to 0.01%!
- · Performance directly indicate behaviour on real survey data
- Recall at low contamination has significantly increased (see ROC curves)

Given class imbalance, still o(10⁴) galaxies to eyeball \rightarrow How can we improve?

Other tests completed

Architecture level: group-invariant network architectures (e.g., Cohen+2016, Schaefer+2018) - networks pre-trained on ImageNet - multiclass classification (e.g., Teimoorinioa+2020)

Data set level: Influence of the number of observing bands - Lens-light subtraction -Masking of neighbouring galaxies -Denoizing image cutouts - Deconvolving image cutouts - combining classification + modeling networks



using observed HSC lenses and non-lenses.

Robustness of neural network classification

Cañameras et al. 2023, arXiv:2306.03136

Has the model based its decision on a spurious correlation in the training data ?



Two pictures labelled as "horse" (Credit: Lapuschkin et al. 2019)

Robustness of neural network classification

Cañameras et al. 2023, arXiv:2306.03136



Interpretability of strong-lens finding neural networks Examples of local methods

To constrain selection functions, improve performance, and identify biases ?

Layer 1

→ Where is the most useful information for lens/nonlens classifications ?

→ Visual inspection of feature maps: Initial vs. later layers (Jacobs+2022)

→ Saliency mapping: Gradient-weighted Class Activation Mapping (Selvaraju+2017)





Layer 2

Layer 4

Interpretability of strong-lens finding neural networks Examples of local methods

To constrain selection functions, improve performance, and identify biases ?

- → Where is the most useful information for lens/nonlens classifications ?
- \rightarrow Sensitivity probes are easy to implement \rightarrow Occlusion mapping (Zeiler & Fergus 2014)
 - Annular masks centered on the central galaxy
 - CNNs "seem to" use relevant information (lensed arcs and multiple images)



Finding rare strong lenses in large data sets Towards automated selections with deep, wide-scale surveys

Network ensembles are very efficient in decreasing false positive rates (Hansen+1990)

- → Individual neural networks learn different representations
- → Ensembles mitigate stochasticity of learning process, and lower the variance in output scores
- → Combine networks, e.g. with different architectures (fixed training data, fixed augmentation)



Architecture	Parameters	CPU hours	TPR	FPR	AUROC	Candidates	Lens	Model reference
BaseNet	581828	104	0.906	0.097	0.973	62 326	13	Andika et al. (2023)
RegNetX002	2338692	1202	0.924	0.072	0.983	160 852	17	Radosavovic et al. (2020)
RegNetY002	2816896	1317	0.899	0.078	0.977	192 797	13	Radosavovic et al. (2020)
Mobile NetV3Large	3 000 484	148	0.938	0.046	0.989	190 808	16	Howard et al. (2019)
EfficientNetB0	4 055 275	314	0.945	0.042	0.991	147 705	19	Tan & Le (2019)
NASNetMobile	4 274 520	434	0.948	0.048	0.991	169 309	17	Zoph et al. (2018)
EfficientNetV2B0	5925012	243	0.958	0.030	0.994	151 319	15	Tan & Le (2021)
ViT-Vanilla	9208772	1185	0.949	0.050	0.990	24 642	16	Dosovitskiy et al. (2020)
ViT-Lite	9 2 3 0 0 6 0	3499	0.960	0.029	0.994	12872	16	Lee et al. (2021)
Xception	20870252	1041	0.970	0.017	0.997	216 620	17	Szegedy et al. (2016)
InceptionV3	21 811 556	549	0.967	0.020	0.996	186 190	17	Szegedy et al. (2015)
ResNet50V2	23579268	1094	0.967	0.021	0.996	164722	18	He et al. (2016)
ResNetRS50	33 705 060	1245	0.966	0.021	0.996	155262	16	Bello et al. (2021)
InceptionResNetV2	54 343 460	1630	0.966	0.014	0.996	150435	18	Chollet (2016)
Ensemble	195 741 135		0.963	0.016	0.996	3080	16	This work

Ensemble classifier for lensed quasar searches in HSC Wide images (Andika+2023)

Finding rare strong lenses in large data sets Towards automated selections with deep, wide-scale surveys

Network ensembles are very efficient in decreasing false positive rates (Hansen+1990)

- → Individual neural networks learn different representations
- → Ensembles mitigate stochasticity of learning process, and lower the variance in output scores
- → Combine networks with different architectures, different ground-truth, data augmentation
 - → Independent networks identify different populations of contaminants



Finding rare strong lenses in large data sets Towards automated selections for deep, wide-scale surveys

Unsupervised learning algorithms

→ For direct, fully-automated classification of strong lenses (Cheng et al. 2020)



Lens finding with (1) a convolutional autoencoder, and (2) a Bayesian Gaussian mixture model (Cheng et al. 2020)

→ Result in elevated contamination rates ...

Finding rare strong lenses in large data sets Towards automated selections for deep, wide-scale surveys

Unsupervised learning algorithms

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Lens finding with (1) a convolutional autoencoder, and (2) a Bayesian Gaussian mixture model (Cheng et al. 2020)

→ For creating large catalogs of non-lens galaxies + retrain a supervised learning algorithm



Finding rare strong lenses in large data sets Towards automated selections for deep, wide-scale surveys

Unsupervised learning algorithms

LRG -0.1 -0.1 -0.0

0.3 0.3 0.3

0.2

0.2

 \rightarrow for deblending image components (Savary+2022), or conducting image denoising (Cheng+2020)?

Residuals

-25.0 0.0 25.0

- 10.0

-10.0

0.0

0.0



L. source

-0.1 -0.1

0.3

0.2

0.3

0.2

Original

0.5

113952+303204

0.5

090129+303355

0.5

164940+304909

1.0

1.0

1.0

0.0

0.0

Image denoizing with a convolutional autoencoder (Cheng+2020)

Lens/source

autoencoder



Schuldt et al. 2021a, A&A 646, A126; Schuldt et al. 2023a, A&A 671, A147

Estimate mass profile parameters

→ Singular Isothermal Ellipsoid + external shear and uncertainties

Regression convolutional neural network

(see also, e.g., Hezaveh+2017, Perreault-Levasseur+2017, Madireddy+2019, Park+2020, Pearson+2019,+2021)





Schuldt et al. 2021a, A&A 646, A126; Schuldt et al. 2023a, A&A 671, A147

Estimate mass profile parameters

Regression convolutional neural network

(see also, e.g., Hezaveh+2017, Perreault-Levasseur+2017, Madireddy+2019, Park+2020, Pearson+2019,+2021)

- **Realistic lens simulations** → Train and test on HSC Wide
- log-probability loss with a regularisation term

$$L = \sum_{k=0}^{N} \sum_{l=0}^{p} \left[-w_l \times P\left(\eta_{k,l}^{\text{pred}}, \eta_{k,l}^{\text{tr}}, \sigma_{k,l}\right) + \epsilon_l \times \log\left(\sigma_{k,l}^2\right) \right]$$
$$P(\eta_{k,l}^{\text{pred}}, \eta_{k,l}^{\text{tr}}, \sigma_{k,l}) = -\frac{\left(\eta_{k,l}^{\text{tr}} - \eta_{k,l}^{\text{pred}}\right)^2}{2\sigma_{k,l}^2} - \ln(\sigma_{k,l}) - \ln(\sqrt{2\pi}).$$







Schuldt et al. 2021a, A&A 646, A126; Schuldt et al. 2023a, A&A 671, A147

Estimate mass profile parameters

Regression convolutional neural network

- Lens mass profile parameters are recovered •
- Results are stable, e.g. for fainter lensed sources •
- Translates into accurate predictions of image positions and time delays



-0.3

evtr

0.3

100

 $\theta_{\rm F}^{\rm tr}$ [arcsec]

-0.3

ey

0.3



0.2

1.0

 $\theta_{\rm E}$ [arcsec]





Schuldt et al. 2023b, A&A 673, A33

Neural network vs traditional modeling

 Use galaxy-scale strong lenses from HSC Wide (Sonnenfeld+2018, Wong+2018) to compare

(1) CNN-based modeling (Schuldt+2023a)

(2) Traditional MCMC sampling-based models with a semi-automated pipeline







Schuldt et al. 2023b, A&A 673, A33

Neural network vs traditional modeling

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Schuldt et al. 2021b, A&A 651, A55

Traditional photo-z codes

- Deblended photometry and fitting of the spectral energy distributions



Directly predict galaxy redshifts from multiband images

- Regression convolutional neural network (d'Isanto+2018, Pasquet+2019, Treyer+2023)
- More systematic pipeline \rightarrow Train and test on HSC Wide grizy to prepare for LSST





Schuldt et al. 2021b, A&A 651, A55



Predict galaxy redshifts from images

- Regression convolutional neural network (d'Isanto+2018, Pasquet+2019, Trever+2023)
 - Data set: galaxies without imaging artifacts and with ground truth redshifts from • (1) spectro surveys, (2) reliable photo-z in COSMOS (30 bands, Laigle+2016)
 - Limit to mag < 25 and Kron radius >0.8" + masking + augmented data set •

0.378: Zurent=0.379

 \rightarrow 10⁵ examples for training a simple CNN





Schuldt et al. 2021b, A&A 651, A55

Predict galaxy redshifts from images

- Training over 0 < z < 4, good performance, larger **bias** at z > 2
- Comparison with DEmP (Hsieh+2014), best method from HSC photo-z team (Nishizawa+2020) → Identical test set













- Supervised machine learning is key to identify rare objects, e.g. strong lenses
- All-sky classification pipeline works, but many contaminants + long visual inspection
- Full automation need systematic network evaluation on external, realistic test sets
 - → Major improvements for specific networks and data sets → FPRs from 1% to 0.01%!
- Some networks learn spurious correlation in the training data \rightarrow Need interpretability
- Ensembles of neural networks leverage diversity of individual models
- Unsupervised machine learning not ready for rare object identification
- ResNet for automated lens modeling + parameter uncertainties → Performance are promising + validated on real strong lens systems
- CNN for automated redshift estimates \rightarrow Competitive approach with broad applications





Bonus slides



Contamination

Cosmology with 6 lensed quasars: H0LiCOW project



Time delays from COSMOGRAIL + Lens modeling + Line-of-sight mass modeling

 \rightarrow H0 with 2.4% precision in flat \land CDM (blind analysis)

Efficient strong lens modeling

Schuldt et al. 2021a, A&A 646, A126



Predict lens mass profile parameters



Schuldt et al. 2021b, A&A 651, A55



Predict photometric redshifts

- Morphological information helps
 - New CNN trained on the same set \rightarrow replacing cutouts with point-like sources
 - Larger scatter + larger bias at higher z

