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Domain-Adaptive Neural Posterior Estimation for Strong Gravitational Lens Analysis

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Abstract

Modeling strong gravitational lenses is prohibitively expensive for modern and next-generation cosmic survey data. Neural posterior estimation (NPE), a simulation-based inference (SBI) approach, has been studied as an avenue for efficient analysis of strong lensing data. However, NPE has not been demonstrated to perform well on out-of-domain target data — e.g., when trained on simulated data and then applied to real, observational data. In this work, we perform the first study of the efficacy of NPE in combination with unsupervised domain adaptation (UDA). The source domain is noiseless, and the target domain has noise mimicking modern cosmology surveys. We find that combining UDA and NPE improves the accuracy of the inference by 1-2 orders of magnitude and significantly improves the posterior coverage over an NPE model without UDA. We anticipate that this combination of approaches will help enable future applications of NPE models to real observational data.

1 Introduction and Related Work

Galaxy-scale strong gravitational lensing is a cosmic probe that provides key information about dark energy, dark matter, and galaxy evolution [4, 96, 95, 66, 49, 34, 94, 86]. Modern and future cosmic survey experiments — e.g., the Dark Energy Survey (DES) [16, 30], Hyper Suprime-Cam [3, 70], the Kilo-Degree Survey (KiDS) [22, 58], the Rubin Observatory Legacy Survey of Space and Time [46], Euclid [27], JWST [83, 13], and the Nancy Grace Roman Telescope [26, 59, 103] — are expected to contain 10^3 - 10^5 lensing systems [74, 87, 17]. Traditional techniques for lens modeling have relied heavily on analytic likelihood-fitting, which is computationally expensive and human-time intensive [61]. Additionally, due to simplifying assumptions in designing the likelihoods, these techniques often lack the capability of modeling non-Gaussian likelihoods and posteriors [61]. However, these techniques have advanced notably in automation and speed [73, 39, 31, 88]. Supervised deep learning-based inference techniques — including neural network regression and the recently reinvigorated simulation-based inference (SBI) [20, 38, 1, 24, 108, 35, 45] like neural posterior estimation (NPE) [75, 36, 102, 107] — have been studied in applications on a wide variety of physics and cosmology topics [21, 51, 79, 80, 8, 41, 64], including strong lensing [47]. Once these models are trained (aka, "amortized"), these methods are very fast compared to traditional modeling methods [20]. In many areas of cosmology, including strong lensing, when there isn't enough real observational data for training deep learning-based models, realistic simulations are used [93, 71, 9, 11]. Nevertheless, these simulated data can differ significantly from real, observational data — i.e., observational noise, astrophysics, and cosmology. The differences between the simulated training data (source domain) and the real observational data used for analysis (target domain) constitute domain shifts between data distributions that can cause models to favor the source domain [90, 99, 67]. Studies of model misspecification due to domain shift [104, 101, 15, 84] have shown this to be a significant limitation of SBI and its application to out-of-domain data. Domain adaptation (DA) is a class of deep learning techniques that help neural networks adapt to domain shifts so that the feature spaces of the source and target domains align during training [106, 97, 111, 109, 56, 60]. Unsupervised domain adaptation (UDA) does not require labels on the target data [105, 57, 85, 110]. This has been studied as an approach to ameliorate biases due to domain shifts for neural network-based analyses in many problems, including cosmology and strong lensing [14, 113, 23, 112, 91, 52, 29, 114, 81, 25, 33, 53]. In this work, we advance the state of the art by combining NPE and UDA and comparing the performance of NPE-UDA and NPE-only models on strong lensing data in two different domains, which are distinguished by the noise in the images.

2 Methods: Lensing, Neural Posterior Estimation, Domain Adaptation

Physics of strong gravitational lensing: When light from a background object encounters a sufficiently massive lensing object on its way to an observer, the image of the background object is significantly magnified and distorted [72, 100]. This warped image is the primary observable data (see Fig. 1(b) for example images). In parametric lens modeling, one can consider > 10 parameters from the background object and the lens that could be inferred from the imaging data [61, 50, 77, 10]. In this study, we infer only five parameters related to the lens: Einstein radius $\theta_{\rm E}$, relative angular positions between the background object and lens (x, y), and lens eccentricity moduli ($e_{\rm l,1}$,$e_{\rm l,2}$). Like all astronomical data, strong lensing images are subject to observational noise from multiple sources — e.g., atmosphere, sky brightness, CCD gain, number of exposures, exposure time, CCD readout, and photon counting. These noises can add values to pixel counts or cause blurring in the images; they need to be accounted for in model building to avoid systematic bias and large error bars.

Neural Posterior Estimation (NPE): To infer parameter posterior densities, we employ NPE [36], which uses a CNN-based embedding network to summarize images into features, which are then passed to a Masked Autoregressive Flow (MAF), a combination of an autoregressive model and a normalizing flow [75], to estimate posterior densities. MAF can estimate posterior distributions of arbitrary shape (i.e., non-Gaussian). In the standard NPE-only approach, there is a single loss function $L_{\rm NPE}$ that takes the form of the negative log posterior volume [36].

Unsupervised Domain Adaptation (UDA): In UDA methods, the source domain data have labels, and the target domain data do not have labels. Common UDA approaches include adversarial methods [91, 69, 40, 54, 48, 32] and distance-based methods [105, 28]. In distance-based methods, the loss is defined as a multi-dimensional distance between latent features from the source and target domain data. In this work, we use distance-based methods, for which the UDA loss function $L_{\rm UDA}$ is the Maximum Mean Discrepancy (MMD) [37]. MMD is a method that calculates the distance between distributions: when applied to the latent feature space, it can be used as a loss function. In [84], MMD was used as a metric to quantify the NPE model misspecification. When MMD is included as a loss during training, it is intended to cause the network to align latent feature spaces for the source and target data; this leads to the extraction of domain-invariant features and enables the model to work well on both.

Combining NPE and UDA: We combine NPE and UDA methods via their losses. The UDA loss $L_{\rm UDA}$ is calculated using the source and target domain latent features (without labels) at the end of the embedding network. The NPE loss $L_{\rm NPE}$ is calculated using the source data (with labels) at the end of the MAF. The total loss function $L_{\rm Tot} = L_{\rm NPE} + \beta_{\rm UDA} * L_{\rm UDA}$ is used with gradient descent to update all weights; $\beta_{\rm UDA}$ is a hyperparameter weighting the MMD loss.

3 Experiments

Data: We use the `deeplenstronomy` [71] software, which is built on `lenstronomy` [9, 11], to generate simulations of galaxy-scale strong lensing images as if observed in a ground-based survey. We use a single photometric band (g), which is sufficient for producing morphological features of a lensing system. Images have a pixel scale of $0.263\,''$/pixel to match that of DES [30, 2]. During

Table 1: Distributions and results for each lensing parameter. The parameters ("params"); **(a)** prior distributions for training and test sets; **(b)** the residuals for the NPE-only and the NPE-UDA models applied to the target domain data; **(c)** the mean residuals for the NPE-UDA model applied to the source domain data.

	(a) Prior Distributions		**(b)** Residual: Target		**(c)** Residual: Source	
Params	Training	Valid/Test	NPE-only	NPE-UDA	NPE-only	NPE-UDA
θ_{E} ($''$)	$\mathcal{U}(0.9, 3.2)$	$\mathcal{U}(1.0, 3.0)$	$-0.05^{+0.18}_{-0.33}$	$-0.006^{+0.045}_{-0.039}$	0.002 ± 0.017	0.000 ± 0.018
x ($''$)	$\mathcal{U}(-1.3, 1.3)$	$\mathcal{U}(-1.0, 1.0)$	-0.06 ± 0.19	0.007 ± 0.076	0.004 ± 0.025	-0.002 ± 0.030
y ($''$)	$\mathcal{U}(-1.3, 1.3)$	$\mathcal{U}(-1.0, 1.0)$	0.07 ± 0.20	0.001 ± 0.079	$-0.001^{+0.021}_{-0.024}$	-0.001 ± 0.030
$e_{\mathrm{l},1}$	$\mathcal{U}(-0.3, 0.3)$	$\mathcal{U}(-0.2, 0.2)$	-0.28 ± 0.75	$0.007^{+0.062}_{-0.075}$	-0.001 ± 0.030	$0.001^{+0.019}_{-0.016}$
$e_{\mathrm{l},2}$	$\mathcal{U}(-0.3, 0.3)$	$\mathcal{U}(-0.2, 0.2)$	0.23 ± 0.62	$0.016^{+0.064}_{-0.084}$	$0.000^{+0.015}_{-0.016}$	$0.004^{+0.015}_{-0.020}$

simulation, the surface brightness of the lensing galaxy is omitted from the images: this exclusion represents a part of the typical lens modeling process in which lens light is removed before the lensed background image is modeled [62]. We use empirically and theoretically motivated uniform priors for distributions of physics parameters of the background object and the lens object. For the background object parameters, which we don't infer, we use the following: Sérsic index $n \sim \mathcal{U}(2, 4)$, scale radius $R \sim \mathcal{U}(0.5'', 1'')$, two-dimensional eccentricity $\{e_{\mathrm{s},1}, e_{\mathrm{s},2}\} \sim \mathcal{U}(-0.2, 0.2)$; two-dimensional external shear $\{\gamma_1, \gamma_2\} \sim \mathcal{U}(-0.05, 0.05)$ [17, 12]. The apparent magnitude of the background object has a distribution $m \sim \mathcal{U}(22.5, 23)$, which is faint enough that the noise will be apparent. For the lens object parameters that we infer (θ_{E}, x, y, $e_{\mathrm{l},1}$, and $e_{\mathrm{l},2}$), the prior distributions are shown in Table 1.

We incur a shift in the domain between the source and the target in terms of image noise characteristics only — i.e., not for the physics parameters. The source data has noise characteristics that represent a relatively noiseless image: read noise is zero e^-, CCD gain is 6.083 e^-/count, exposure time is 90 seconds (typical modern optical cosmic surveys), number of exposures is 10, magnitude zero point is 30, sky brightness is 23.5 magnitude/arcsec^2 (dimmer than the source light profile), and seeing is $0.9''$ (moderate for modern optical cosmic surveys). In contrast, the target data has noise characteristics that mimic those of the DES: read noise is 7.0 e^-, and exposure time, number of exposures, magnitude zero point, sky brightness, and seeing are sampled from empirical distributions [2]; these distributions are encoded in the `deeplenstronomy` package.

The training set contains 200,000 images in each domain — source and target. These are drawn from the training priors. The validation and test sets each contain 1,000 images in each of the domains. These are drawn from the test priors. The $\texttt{sbi}_{\text{Macke}}$ package holds out 10% of the training data for validation during training and early stopping; that validation set is independent of the one we created. For the lens parameters that we infer, the prior distributions for training are wider than the prior distributions for testing to mitigate biases near the edges of the test distribution (see Table 1). The test set is used for all results and metrics in this paper. Sample lenses from source and target data are shown in Fig. 1(b). All images are 32×32 pixels in shape. The data set uses $\sim$ 3.5 GB of storage space. The data used in this project can be provided upon request.

Model Optimization: We use the $\texttt{sbi}_{\text{Macke}}$ package [92], which utilizes PyTorch [76] to perform NPE analyses. For the NPE model, we use an embedding network to summarize the image data before input to the MAF. The embedding network architecture has six convolution blocks (each with a convolution, max-pooling, and batch normalization layer) followed by one dropout (rate is 0.5) and one dense layer with 20 nodes. The MAF has 20 transformation blocks, with 400 hidden features in each. This NPE architecture was introduced in [78]. We experimented with a variety of hyperparameter choices and data sets. We determined that the $\texttt{sbi}_{\text{Macke}}$ package defaults most clearly show the models' performances: the batch size, learning rate, optimizer, and early stopping epochs are 50, 0.0005, `Adam` optimizer [55], and 20, respectively. We set $\beta_{\text{UDA}} = 1.0$. We discuss computational costs for model training in Appendix F. The code for this work can be provided upon request.

4 Results: UDA improves NPE performance on target domain data

First, we check that the addition of UDA to NPE does not lead to a significant deterioration in model performance on source data compared to NPE alone. For all parameters, the NPE-UDA model is slightly more accurate when applied to the source data than when applied to the target data (Fig. 1(a) and Table 1(c)). Also, the NPE-UDA model has nearly the same degree of calibration on source data as on target data (Fig. 1(d)). Next, the demonstration of performance relies on comparing the NPE-only and NPE-UDA models on target data. The NPE-only model has an average residual (i.e., bias) of $0.26''$ for the Einstein radius. This bias is far outside the state-of-the-art uncertainties for traditional modeling techniques, which produce uncertainties at the level of $\sim 0.01''$ [65] or, more generally, at $\sim$ 1-5% [82, 89]. In contrast, for the NPE-UDA model, the accuracy improves (the average residual reduces) by approximately 88%, 88%, 99%, 98%, and 93% for all five parameters $\theta_{\rm E}$, $e_{\rm l,1}$, $e_{\rm l,2}$, x, y, respectively. Also, in applications to the target domain data, the parameter uncertainties for the NPE-UDA model are very well-calibrated, while those for the NPE-only model are highly overconfident (Fig. 1(d)). This reflects the NPE-only model's bias toward the source domain when applied to the target domain data. Finally, the feature spaces for the NPE-UDA model applied to source and target data are overlapping but not when the NPE-only model is applied to data from those domains (Fig. 1(b) left and right, respectively).

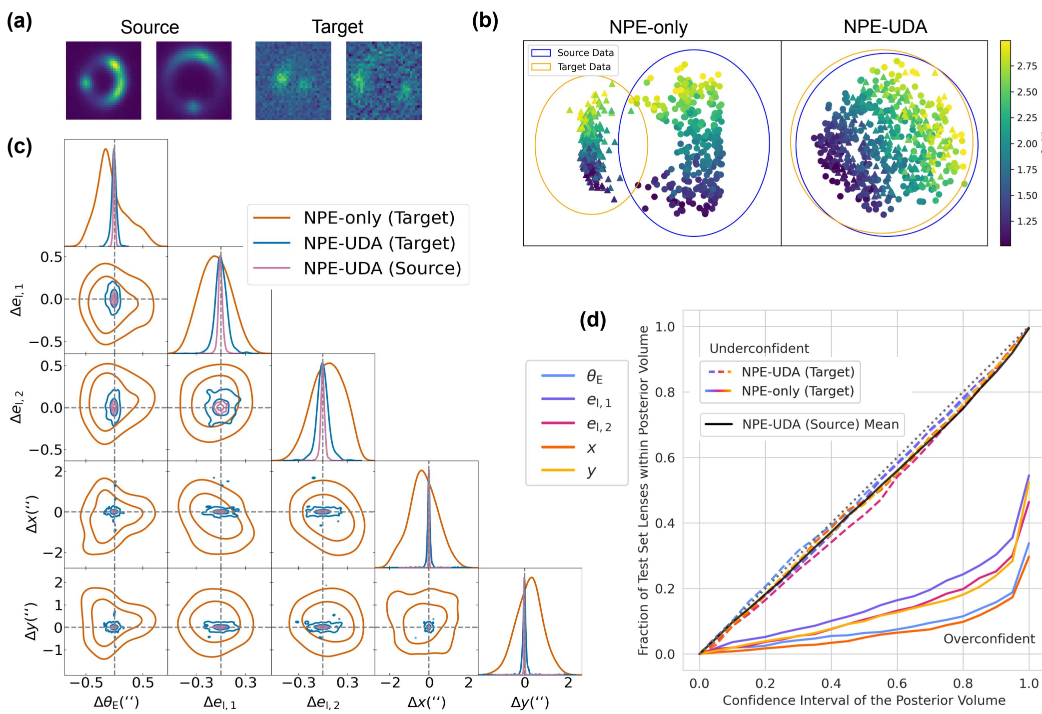

Figure 1: (**a**): Two example images from the source (without noise; left) and target (with noise; right) domains. (**b**): Feature spaces of the embedding network when models are applied to the source (points are filled circles; all points encompassed by a blue circle) and target (points are filled triangles; all points encompassed by an orange circle) domain data for the NPE-only (left) and NPE-UDA (right) models, respectively. (**c**): Residuals on the five lens parameters ($\theta_{\rm E}$, x, y, $e_{\rm l,1}$, $e_{\rm l,2}$) for the NPE-only model applied to target data (orange), the NPE-UDA model applied to target data (blue), and the NPE-UDA model applied to source data (pink). Contours show the 68th- and 95th-percentile confidence regions, and the dashed lines show zero residuals. (**d**): Posterior coverage on the five lens parameters for the NPE-only model for the NPE-UDA model applied to target data (dashed, color), the NPE-only model applied to target data (solid, color), and the NPE-UDA model applied to source data (solid, black). The boundary between underconfident (upper) and overconfident (lower) is marked by a dotted gray line.

5 Summary and Outlook

We show for the first time that (unsupervised) domain adaptation (UDA) enhances simulation-based inference (SBI) models when applied to unlabeled target domain data. We used neural posterior estimation (NPE) to infer five parameters of lensing systems from single-band imaging data. We compare NPE models that have UDA (NPE-UDA) to NPE models that don't have UDA (NPE-only) (§2). We incurred a domain shift between the source and target domains: the source images are nearly noiseless, and the target images have the same noise characteristics as DES (§3). When applied to the target domain, the NPE-UDA model is 1-2 orders of magnitude more accurate than the NPE-only model for all five lens parameters (Fig. 1(c) and Table 1(b)). Similar approaches may significantly improve the accuracy of SBI/NPE models when they are applied to real observational data.

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B Author Contributions

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Ćiprijanović: Conceptualization, Methodology, Formal analysis, Writing - Review & Editing, Supervision, Project administration

Nord: Conceptualization, Methodology, Formal analysis, Resources, Writing - Original Draft, Writing - Review & Editing, Supervision, Project administration, Funding acquisition

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C Attributions: Software and Computing Facilities

We used the following software packages: `Astropy` [7, 5, 6], `deeplenstronomy` [71], `Elastic Analysis Facility (EAF)` [43], `Getdist` [63], `H5py` [18], `lenstronomy` [9, 11], `Matplotlib` [44], `Numpy` [42], `Python` [98], `PyTorch` [76], $\texttt{sbi}_{\text{Macke}}$ [92], `Torch` [19], `Torchvision` [68].

D Embedding Network

We use an embedding network to reduce the feature space of the imaging data before the MAF uses it. See Table 2 for the architecture setup, including hyperparameters.

E Additional Feature Space Inspection

In the main text, we showed that the feature spaces for the NPE-UDA model on the source and target domains are well-aligned (§4 and Fig. 1(b)) for Einstein radius, and there is a clear monotonic correlation between the feature space and the Einstein radius magnitude. Here, we further inspect

Table 2: The architecture of the embedding network used in the NPE to compress the image data into summary features. The first column lists the layer type, the second column lists the dimensionality of the output from that layer, and the third column lists the parameters of that layer; k is the kernel size, and s is the stride. The final layer outputs the summary features.

Layer	Output shape	Parameters
Conv2d	[-1, 8, 32, 32]	$k = 3$, $s = 1$
BatchNorm2d	[-1, 8, 32, 32]	$k = 3$, $s = 1$
Conv2d	[-1, 16, 32, 32]	$k = 3$, $s = 1$
BatchNorm2d	[-1, 16, 32, 32]	$k = 3$, $s = 1$
MaxPool2d	[-1, 16, 16, 16]	$k = 2$, $s = 2$
Conv2d	[-1, 32, 16, 16]	$k = 3$, $s = 1$
BatchNorm2d	[-1, 32, 16, 16]	$k = 3$, $s = 1$
Conv2d	[-1, 32, 16, 16]	$k = 3$, $s = 1$
BatchNorm2d	[-1, 32, 16, 16]	$k = 3$, $s = 1$
MaxPool2d	[-1, 32, 8, 8]	$k = 2$, $s = 2$
Conv2d	[-1, 64, 8, 8]	$k = 3$, $s = 1$
BatchNorm2d	[-1, 64, 8, 8]	$k = 3$, $s = 1$
Conv2d	[-1, 128, 8, 8]	$k = 3$, $s = 1$
BatchNorm2d	[-1, 128, 8, 8]	$k = 3$, $s = 1$
MaxPool2d	[-1, 128, 4, 4]	$k = 2$, $s = 2$
Flatten	[-1, 2048]	-
Linear	[-1, 20]	-

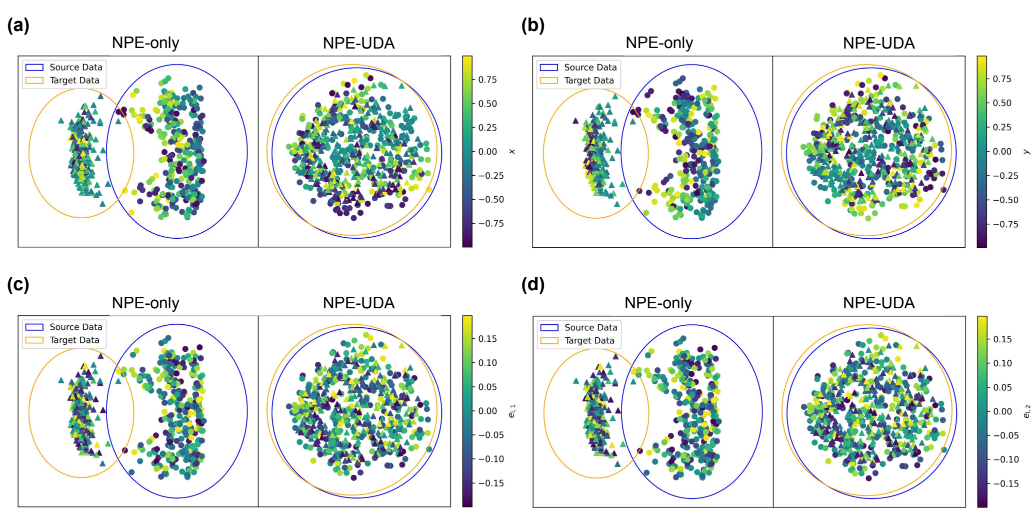

Figure 2: Latent space of the embedding network when NPE is applied to the source and target domain test set data for the NPE-only (left) and NPE-UDA (right) models, respectively. This is applied to parameters x **(a)**, y **(b)**, $e_{1,1}$ **(c)**, $e_{1,2}$ **(d)**.

the feature spaces for the NPE-only and NPE-UDA models on the relative positions x and y, and on the lens eccentricity moduli $e_{1,1}$ and $e_{l,2}$. A non-monotonic correlation exists between the feature space and the parameter of interest for x and y, but not for the lens eccentricities. We experimented with the isomap hyperparameter for the number of neighbors (default is five), and we found that values greater than 20 did not change the visualization. We speculate that while the NPE-UDA model requires the feature spaces to overlap, it prioritizes the correlation with the Einstein radius over other parameters. Additionally, the other parameters are more subtly represented in the images and thus may be more difficult to learn.

F Computational costs for experiments

All computing was executed on an NVIDIA A100 GPU with 10GB memory. These computations were performed on the Fermilab Elastic Analysis Facility [EAF; 43]. Training without UDA requires ~ 4.0 hours, while training with UDA requires ~ 6.5 hours. This additional time is primarily due to a) calculating the additional loss function for UDA and b) using twice the amount of data by including the target domain data.