Neural network prediction of strong lensing systems with domain adaptation and uncertainty quantification

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Abstract

Modeling strong gravitational lenses is computationally expensive for the complex data from modern and next-generation cosmic surveys. Deep learning has emerged as a promising approach for finding lenses and predicting lensing parameters, such as the Einstein radius. Mean-variance Estimators (MVEs) are a common approach for obtaining aleatoric (data) uncertainties from a neural network prediction. However, neural networks have not been demonstrated to perform well on out-of-domain target data successfully — e.g., when trained on simulated data and applied to real, observational data. In this work, we perform the first study of the efficacy of MVEs in combination with unsupervised domain adaptation (UDA) on strong lensing data. The source domain data is noiseless, and the target domain data has noise mimicking modern cosmology surveys. We find that adding UDA to MVE increases the accuracy on the target data by a factor of about two over an MVE model without UDA. Including UDA also permits much more well-calibrated aleatoric uncertainty predictions. Advancements in this approach may enable future applications of MVE models to real observational data.

1 Introduction and Related Work

Strong gravitational lensing provides critical insights into galaxy evolution, dark matter, and dark energy [4, 112, 111, 72, 57, 41, 110, 100]. Modern cosmological surveys [20, 35, 3, 81, 24, 60, 55, 32, 98, 15, 29, 62, 119] are expected to contain 10^3 - 10^5 lensing systems [85, 102, 21]. Traditional lens finding techniques have relied heavily on human-intensive image reviewing [87, 86, 94, 95, 77], and modeling has relied on computationally-intensive analytic likelihood-fitting [13, 65, 58, 27, 31]. This has motivated supervised deep learning-based techniques like neural network classification and regression to be applied to strong lensing in addition to a wide variety of cosmology topics [80, 105, 49]. Obtaining uncertainties is important for these areas of study [68]. They can be obtained in network regression through a variety of methods — e.g., MC Dropout [36, 47, 116, 64], Bayesian Neural Networks [BNNs; 19, 18, 8, 114, 43], mean-variance estimation [103, 109, 25, 106], Deep Ensembles [17, 40, 106, 63, 28, 37, 2], Deep Evidential Regression [124, 79, 78, 6], and Simulation-Based Inference [23, 66, 67, 117]. Once trained, these methods are typically very fast compared to traditional parametric modeling methods [68]. However, all of these models face the challenge that there is insufficient observational data for training and instead rely on realistic simulations [12, 82, 5, 70, 91, 93, 92].

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Despite the realism, simulated data can differ from real, observational data — e.g., the image noise parameters, the range of astrophysics parameters, or the range of cosmology parameters. Sometimes, real data is used directly in training [52, 53] or is combined with simulated data [125]. The differences between the training data (source domain data) and the real observational data (target domain data) constitute domain shifts between data distributions that cause models to favor the source (training) data [69, 51, 127]. Typically, this problem arises when there are few or no labels for the target data for the model to train on [122, 59]. 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 data domains align when the domain-adapted model is applied [34, 48, 30, 83, 126, 128]. Unsupervised domain adaptation (UDA) is a subclass of techniques that use unlabeled target data [33, 123, 73]. Studies have explored DA in many fields, including cosmology and strong lensing [96, 134, 113, 130, 129, 131, 133, 132, 7, 118]. In this work, we combine MVE and UDA and compare the performance of MVE-UDA and MVE-only models on strong lensing data in two domains that are distinguished by the noise in the images.

2 Methods: Lensing, Mean-variance Networks, and Domain Adaptation

Physics of strong lensing: Galaxy-scale strong lensing occurs when a foreground lens galaxy deflects light from a background galaxy, creating a magnified and warped image of the background object. This distorted image is the primary observable (Fig. 1(a)) for predicting physics parameters. Multiple kinds of noise sources — e.g., atmosphere, sky brightness, CCD readout, and photon counting — can further distort the image. The Einstein radius θ_{E} indicates the spatial scale of the lensing system and depends on the lens galaxy mass distribution, which is complex but can often be modeled with a 5-parameter singular isothermal ellipsoid (SIE), including the Einstein radius [84]. We predict θ_{E}.

Mean-variance Estimation Networks: Mean-variance Estimators (MVEs) estimate the mean and variance of data labels, where the variance is the square of the aleatoric uncertainty σ_{al} [103, 25, 99]. The MVE loss function is set to the β-negative log-likelihood: $L_{\mathrm{MVE}} = \mathcal{L}_{\beta-\mathrm{NLL}}(\beta_{\mathrm{NLL}})$, where β_{NLL} is a hyperparameter. For the NLL loss, the gradient becomes small for high-variance data points, causing them to be undersampled. The β-NLL approach resolves this by multiplying a variance-re-weighting term $\sigma^{2\beta_{\mathrm{NLL}}}$ [99]. For $\beta_{\mathrm{NLL}} = 1$, the gradient is equivalent to that for the mean-squared error (MSE) loss. For $\beta_{\mathrm{NLL}} = 0$, the original NLL loss is recovered.

Unsupervised Domain Adaptation (UDA): In UDA, the source data have labels, while the target data do not have labels. Common UDA approaches include adversarial methods [74, 42, 38, 39] and distance-based methods [44, 61, 107, 122]. We use the distance-based method, Maximum Mean Discrepancy (MMD), wherein the loss L_{UDA} is a multi-dimensional distance between latent embeddings of the source and target data sets [44, 108]. In minimizing the MMD loss, these embeddings of the source and target data become aligned and include domain-invariant features, which allows the model to perform well on domain-shifted data.

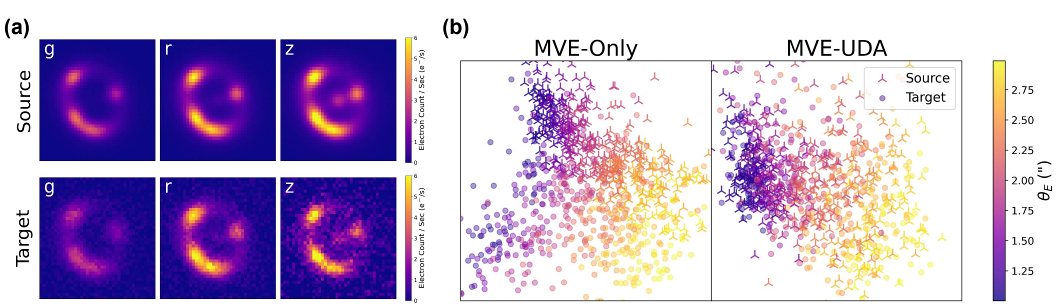

Figure 1: **(a)**: Example lensing images in the source domain (top) and the target domain (bottom) in bands g, r, and z. **(b)**: Isomaps of the latent space embeddings when the MVE-only model (left) and the MVE-UDA model (right) are applied to the source (triplet) and target (circle) domain data.

Combining MVE and UDA: We combine these two methods via their loss functions. First, the source and target data are both passed through convolutional layers. UDA loss is then calculated on the source and target domain latent embedding — i.e., the layer where extracted features are flattened into one dimension. Then, the source domain embedding is passed into dense layers, and the MVE

Table 1: Prior distributions of the simulation parameters for training and test sets.

Parameter		Prior
Lens light profile		
Einstein radius	$\theta_{\rm E}$ ($''$)	$\mathcal{U}(1.0, 3.0)$
Sérsic index	n	$\mathcal{U}(2.0, 5.0)$
Scale radius	R ($''$)	$\mathcal{U}(1.0, 2.5)$
Eccentricity	$\{e_{\rm l,1}, e_{\rm l,2}\}$	$\mathcal{U}(-0.2, 0.2)$
External shear	$\{\gamma_1, \gamma_2\}$	$\mathcal{U}(-0.05, 0.5)$
Source light profile		
Sérsic index	n	$\mathcal{U}(2.0, 4.0)$
Scale radius	R ($''$)	$\mathcal{U}(0.5, 1.0)$
Eccentricity	$\{e_{\rm s,1}, e_{\rm s,2}\}$	$\mathcal{U}(-0.2, 0.2)$
Relative angular positions	$\{x, y\}$ ($''$)	$\mathcal{U}(-0.5, 0.5)$

loss is calculated on the source data only. The total loss is $L_{\rm Tot} = \mathcal{L}_{\beta-\rm NLL}(\beta_{\rm NLL}) + \alpha_{\rm UDA} * L_{\rm UDA}$, where $\alpha_{\rm UDA}$ determines the weight of the UDA loss relative to the MVE loss. The total loss is used to update all weights.

3 Experiments

Data: We use the `deeplenstronomy` [82, 12, 14] to simulate ground-based telescope images of galaxy-scale strong lenses. Images have a pixel scale $0.263''$/pixel, matching the Dark Energy Survey (DES) [1]. The lens galaxy light profile (Sérsic) is assumed to be centered on the lensing mass. We use theoretically and empirically inspired uniform priors for typical strong lensing parameter distributions. For the lens mass, we use SIE profile, Einstein radius $\theta_{\rm E}$, eccentricity $\{e_{\rm l,1}, e_{\rm l,2}\}$, and external shear $\{\gamma_1, \gamma_2\}$ [84]. Two-dimensional source eccentricity is $\{e_{\rm s,1}, e_{\rm s,2}\}$. For the lens and source light profiles, we use Sérsic profiles with distribution index n, and scale radius R. The relative angular positions between the background and lens galaxies are $\{x, y\}$. Prior ranges for all simulation parameters can be found in Table 1.

We use three photometric bands (g, r, z) to get rich image morphologies during training. To generate realistic galaxy colors, each simulated lens galaxy is assigned a redshift in the range $z_l < 0.7$, and each background galaxy a redshift in the range $1.27 < z_s < 2$ according to the DES Y3 Gold Catalog [101, 125]. Each galaxy is randomly assigned a color from a real galaxy according to the assigned redshift [26]. So that each lens galaxy is visible but not saturated, we use a lower limit on the apparent magnitude for all bands ($\{m_g, m_r, m_z\} > 17.5$) and an upper limit for any one of the bands ($\{m_g, m_r, m_z\} < 21$). For the background galaxy, we use the limits $\{m_g, m_r, m_z\} > 17.5$ and $m_g < 22$ [125]. Redshifts are used solely for colors and are independent of the lensing configuration.

We induce a domain shift between the source and the target domains in terms of image noise. The source data has noise characteristics that represent a nearly noiseless image: read noise is 0 e^-; no sky brightness is added; the exposure time is 1000 seconds (set high to minimize Poisson/shot noise); the number of exposures is 10; the zero-point magnitude is 30; the CCD gain is 6.083 e^-/count; seeing is $0.9''$ (moderate for modern optical cosmic surveys) [1, 45, 82]. In contrast, the target data has noise that mimics DES: the read noise is 7.0 e^-, the exposure time is 90 seconds (typical of modern optical cosmic surveys) [1, 26], and the number of exposures, the magnitude zero point, the sky brightness, and the seeing are sampled from empirical distributions [1]. Our dataset has 100,000 objects each for the source and target data. We use a 70/10/20 (training/validation/test) split for all data. The test set is used for all results in this paper. All images have a shape of 40$\times$40 pixels. The dataset uses $\sim$ 9 GB. Project data can be found on Zenodo. An example image is shown in Fig. 1(a).

Model Optimization: We build our models using `PyTorch` [89]. The network has three convolution blocks (each with a convolution, maxpooling, and batch normalization layer) followed by three dense layers with 128, 32, and two nodes, respectively. MVE techniques present challenges for training — e.g., highly fluctuating loss functions [99]. We found that a batch size of 128, a learning rate of 0.001, and default settings for `AdamW` provided optimal model performance [75]. We considered scheduling of the hyperparameters for the UDA and MVE losses. We found the best results with $\beta_{\rm NLL} = 0.5$ [99] and $\alpha_{\rm UDA} = 1.4$. Over 150 epochs of training, we selected the best model as the one that minimized the MVE loss on source data. For some seeds, the MVE-UDA model pathologically predicts a mean or variance of zero and does not recover — further investigation of this is out of scope. Appendix D briefly discusses architecture and training details. Project code can be found on Github.

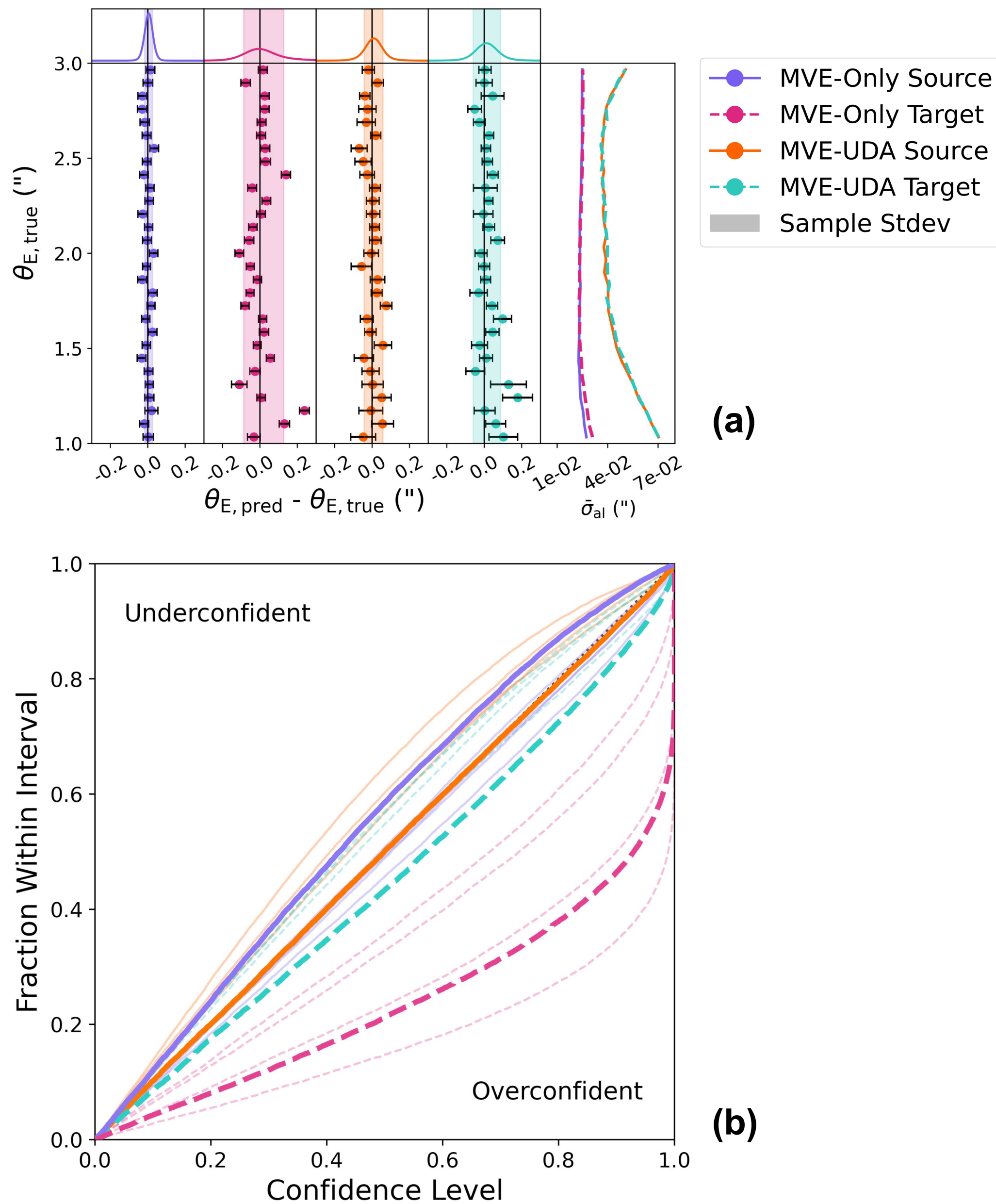

Figure 2: **(a)**: The four left plots show the residuals of the Einstein radius inference for the MVE-only model on the source data (purple, solid), the MVE-only model on the target data (pink, dashed), the MVE-UDA model on the source data (orange, solid), and the MVE-UDA model on the target data (cyan, dashed). The points and error bars are the residuals from the means and the aleatoric uncertainties for randomly selected objects from the test set in each domain. The sample standard deviation is shaded with the corresponding color for each plot. The fifth (right) plot shows the binned average aleatoric uncertainty $\bar{\sigma}_{\mathrm{al}}$. **(b)**: Uncertainty coverage on the Einstein radius for the MVE-only and MVE-UDA models applied to source and target data for five randomly seeded models. The bold lines highlight the Selected model. Panels **(a)** and **(b)** share the same colors and line styles.

Table 2: Mean residual $\langle\delta\theta_{\mathrm{E}}\rangle$ and mean aleatoric uncertainty $\langle\sigma_{\mathrm{al}}\rangle$ of the for the "Selected" Model; the "Median" $\langle\delta\theta_{\mathrm{E}}\rangle_{\mathrm{med}}$ and $\langle\sigma_{\mathrm{al}}\rangle_{\mathrm{med}}$ across five MVE-only and five MVE-UDA model fits. The units are arcsec ($''$). Calculations are described in §4. Appendix E briefly discusses quantities for the four other models.

	Selected				Median			
	(a) Residual $\langle\delta\theta_{\mathrm{E}}\rangle$		**(b)** Uncertainty $\langle\sigma_{\mathrm{al}}\rangle$		**(c)** Residual $\langle\delta\theta_{\mathrm{E}}\rangle_{\mathrm{med}}$		**(d)** Uncertainty $\langle\sigma_{\mathrm{al}}\rangle_{\mathrm{med}}$	
Model	Source	Target	Source	Target	Source	Target	Source	Target
MVE-only	0.0201	0.0818	0.0243	0.0253	0.0164	0.0585	0.0203	0.0205
MVE-UDA	0.0358	0.0425	0.0489	0.0503	0.0389	0.0461	0.0628	0.0628

4 Results: UDA improves MVE performance on the target domain

We trained five models that differed in their weight initialization. The median results across initializations are consistent with the "Selected" model (Table 2). Therefore, unless otherwise stated, we refer only to results of the "Selected" model for clarity of presentation. For the mean residual $\langle\delta\theta_{\mathrm{E}}\rangle = \langle\theta_{\mathrm{E,pred}} - \theta_{\mathrm{E,true}}\rangle$ and aleatoric uncertainty $\langle\sigma_{\mathrm{al}}\rangle$, we take the mean over all the data for a single model. Ideally, the successful combination of MVE and UDA (MVE-UDA) would perform comparably to the MVE-only model on the source data. When applied to source data, the MVE-UDA model has a higher mean residual $\langle\delta\theta_{\mathrm{E}}\rangle$ by $\sim 0.015''$ compared to the MVE-only model (Table 2(a), Fig. 2(a; four left plots)). The mean uncertainty of the MVE-UDA model is approximately twice that of the MVE-only model (Table 2(b), Fig. 2(a; fifth, right plot)). At the same time, the MVE-UDA model is better calibrated (less underconfident) than the MVE-only model (Fig. 2(b)). For target data, however, the MVE-only model has a high mean residual $\langle\delta\theta_{\mathrm{E}}\rangle = 0.0818''$, twice the MVE-UDA model's mean residual $\langle\delta\theta_{\mathrm{E}}\rangle = 0.0425''$ (Table 2(a)). In contrast, the MVE-only model has a low mean uncertainty $\langle\sigma_{\mathrm{al}}\rangle = 0.0253''$, half the MVE-UDA model's mean uncertainty $\langle\sigma_{\mathrm{al}}\rangle = 0.0503''$ (Table 2(b)). Commensurately, the MVE-only model is significantly overconfident, while the MVE-UDA model is only slightly overconfident (Fig. 2(b)) on target data.

The MVE-UDA model uncertainty is higher at both low and high values of θ_{E} (Fig. 2(a) and Fig. 2(a; fifth, right plot))). The high uncertainty for the MVE-UDA model at low θ_{E} may be due to low image resolution or high seeing, such that smaller lensing arcs could be obscured. The high uncertainty at high θ_{E} may be caused by the image being too small to contain the lensing arcs. The residuals and uncertainties for both models are slightly larger than uncertainties assumed in some studies $\sim 0.01''$ [71] but comparable to those from traditional modeling techniques $\sim$ 1-5% [97, 104]. In Fig. 1(b), we find that the target and source embeddings do not overlap for the MVE-only model. In contrast, the embeddings overlap almost completely for the MVE-UDA model, and the points exhibit a gradient in the Einstein radius. These items indicate that the embedding vectors of both are correlated with θ_{E}, but only the MVE-UDA embedding has accurate alignment across domains. Lastly, the coverage of the MVE-only model varies significantly on the target data across initializations, but performance is stable for MVE-UDA (Fig. 2(b)). We find DA is essential to MVE for better calibrated, consistent, and accurate performance on domain-shifted datasets.

5 Summary and Outlook

In this work, we provide the first demonstration that unsupervised domain adaptation (UDA) significantly improves the performance of mean-variance estimator (MVE) models on unlabeled target data. We predicted the Einstein radius of strong gravitational lenses with MVEs (§2). We incurred a domain shift between the source and target domains so that the source images are approximately noiseless, and the target images have noise characteristics similar to DES (§3). When applied to the noisy target data, the MVE-UDA model is significantly better calibrated, more consistent across weight initialization, and more accurate than the MVE-only model (Fig. 2(a) and Table 2(c,d)). Similar approaches may improve neural network model performance when applied to real, observational data.

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B Author Contributions

Agarwal: Methodology, Formal analysis, Software, Validation, Data Curation, Investigation, Writing - Original Draft

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 Software Attribution

We used the following software packages: `Astropy` [11, 9, 10], `deeplenstronomy` [82], `lenstronomy` [12, 14], `Matplotlib` [54], `Numpy` [46], `Pandas` [88] `Python` [115], `PyTorch` [89], `Scipy` [56, 121], `Seaborn` [120], `Sklearn` [16, 90], `Torch` [22], `Torchvision` [76],

D MVE Network Architecture

See Table 3 for the detailed MVE network architecture. There are 112,866 trainable parameters. We note that the activation function for the final dense layers is chosen to be sigmoid rather than ReLU, since ReLU predicts a value of zero for any negative input, encouraging predictions of zero mean or variance. This issue can also be solved by alternative approaches, such as the use of Leaky ReLU or other activation functions that disincentivize a prediction of zero.

E Model inference with varied weight initializations

We performed experiments five times, each with a different random seed for the network weight initialization. All models received the same optimization procedure (§3). The performance of MVE-only model on the target data sets is inconsistent across the seed choices. In contrast, the MVE-UDA model performs consistently slightly worse than the MVE-only model on the source data

Table 3: The architecture of the MVE network. The first column lists the layer type, the second 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 mean and variance.

Layer	Output shape	Parameters
Conv2d	[-1, 8, 40, 40]	$k = 3$, $s = 1$
BatchNorm2d	[-1, 8, 40, 40]	$k = 3$, $s = 1$
MaxPool2d	[-1, 8, 20, 20]	$k = 2$, $s = 2$
Conv2d	[-1, 16, 20, 20]	$k = 3$, $s = 1$
BatchNorm2d	[-1, 16, 20, 20]	$k = 3$, $s = 1$
MaxPool2d	[-1, 16, 20, 20]	$k = 2$, $s = 2$
Conv2d	[-1, 32, 10, 10]	$k = 3$, $s = 1$
BatchNorm2d	[-1, 32, 10, 10]	$k = 3$, $s = 1$
MaxPool2d	[-1, 32, 5, 5]	$k = 2$, $s = 2$
Linear	[-1, 128]	-
Linear	[-1, 32]	-
Linear	[-1, 2]	-

across varied weight initialization. However, unlike the MVE-only model, it consistently performs equally well on the target data as on the source data. This indicates UDA adds stability against the domain shift and is necessary for the application of MVE to datasets with a domain shift. For some initializations, the MVE-UDA model training starts with predictions of zero for the mean or variance, which is erroneous. Further training does not improve the performance. Investigating this pattern in detail is outside the scope of this work. We chose seeds where this pathological behavior does not occur in the first epoch of training.

F Computational costs for experiments

All computing was executed on an NVIDIA A100 GPU with 40GB memory. These computations were performed on the Fermilab Elastic Analysis Facility [EAF; 50]. Training with and without UDA require the same amount of time, ~ 2.5 hours.

Table 4: Mean residual $\langle \delta\theta_{\mathrm{E}} \rangle$, mean aleatoric uncertainty $\langle \sigma_{\mathrm{al}} \rangle$, mean correlation coefficient $\langle R^2 \rangle$, and mean NLL loss $\langle \mathcal{L}_{\beta-\mathrm{NLL}} \rangle$ across each data set for each model, MVE-only, MVE-UDA.

		MVE-only		MVE-UDA	
Metric	Seed	Source	Target	Source	Target
Residual: $\langle \delta\theta_{\mathrm{E}} \rangle$	56	0.0164	0.0693	0.0358	0.0436
	11	0.0149	0.0287	0.0389	0.0425
	31	0.0201	0.0585	0.0386	0.0461
	6	0.0150	0.0818	0.0484	0.0510
	63	0.0174	0.0240	0.0452	0.0551
Uncertainty: $\langle \sigma_{\mathrm{al}} \rangle$	56	0.0243	0.0253	0.0489	0.0503
	11	0.0180	0.0179	0.0602	0.0599
	31	0.0269	0.0239	0.0634	0.0634
	6	0.0192	0.0199	0.0678	0.0678
	63	0.0203	0.0205	0.0628	0.0628
Correlation: $\langle R^2 \rangle$	56	0.9986	0.9642	0.9924	0.9835
	11	0.9988	0.9939	0.9917	0.9897
	31	0.9979	0.9727	0.9922	0.9886
	6	0.9988	0.9418	0.9880	0.9861
	63	0.9984	0.9968	0.9889	0.9832
NLL Loss: $\langle \mathcal{L}_{\beta-\mathrm{NLL}} \rangle$	56	-3.3603	4.5586	-2.6600	-2.4204
	11	-3.4737	-1.0705	-2.5098	-2.4385
	31	-3.1443	15503.4180	-2.4316	-2.2854
	6	-3.4925	25.4278	-2.2687	-2.2070
	63	-3.2745	-2.6643	-2.2982	-2.0623