Distribution-Informed Neural Networks for Domain Adaptation Regression

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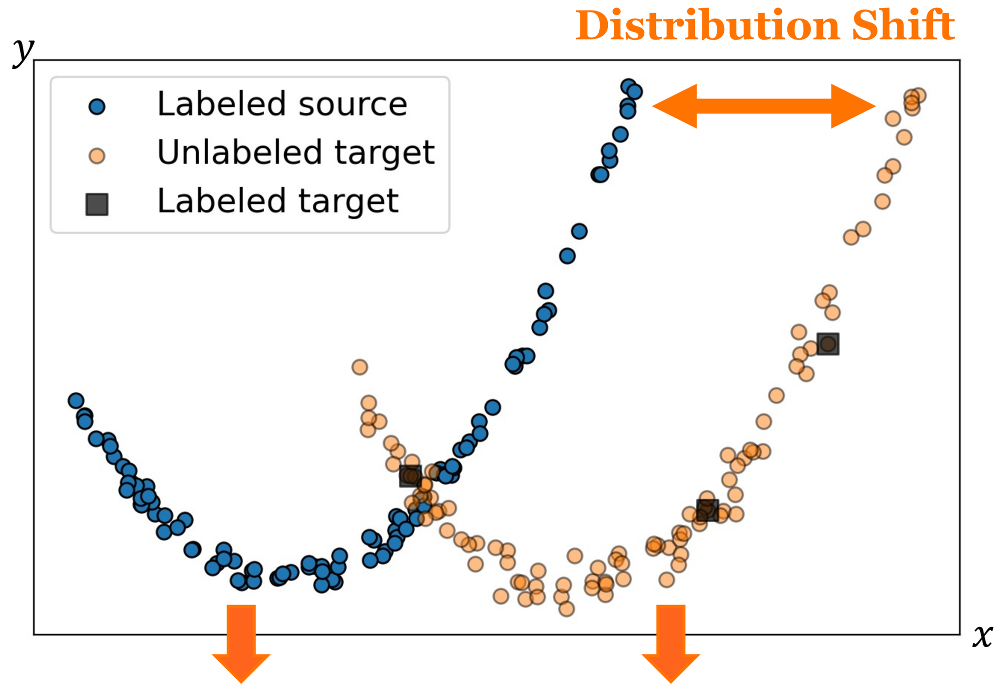
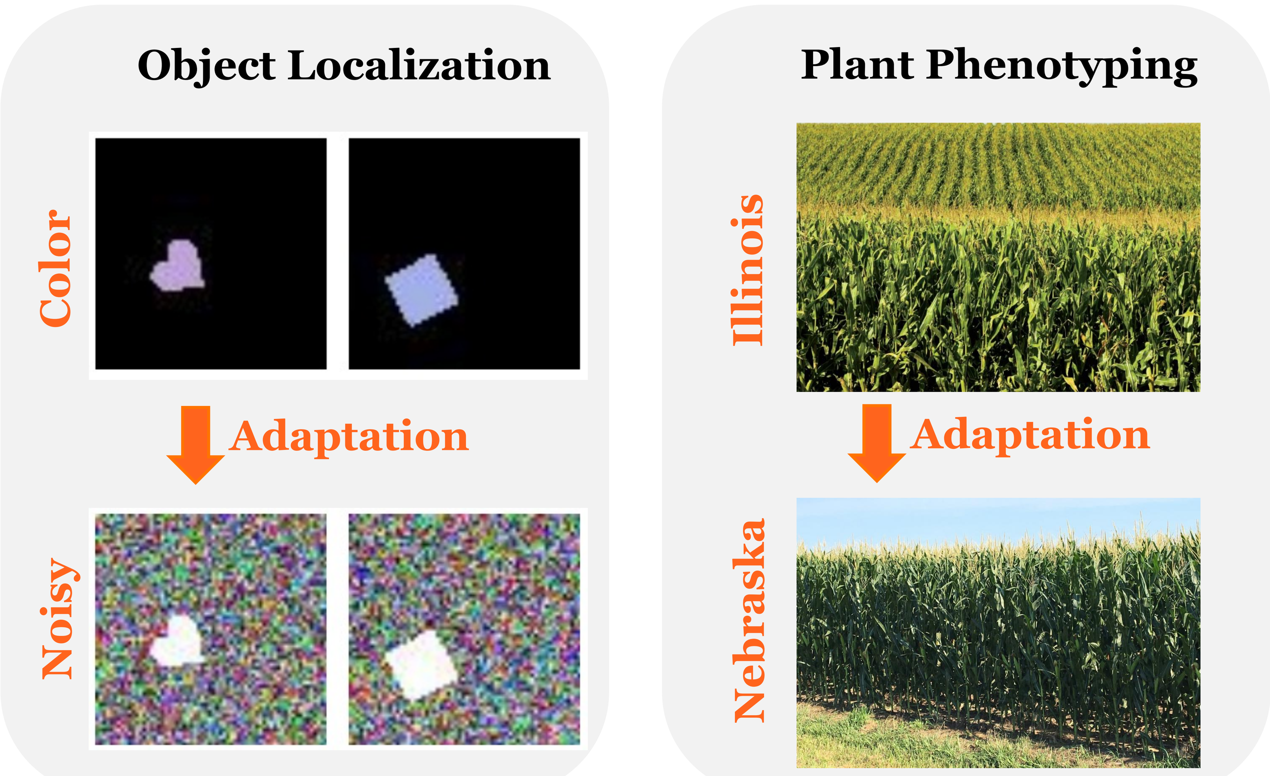
AIFARMS Artificial Intelligence for Future Agricultural Resilience, Management, and Sustainability

Background

❑ Domain adaptation regression



❑ Applications

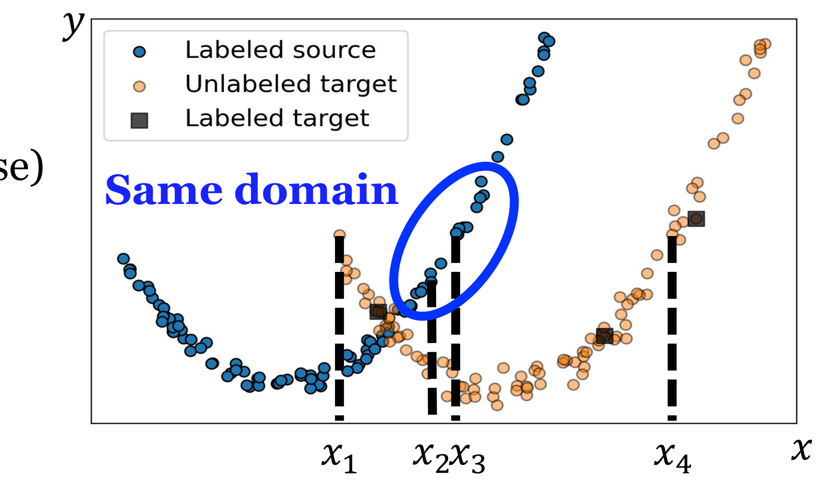


Distribution-Informed Neural Network (DINO)

❑ Motivation

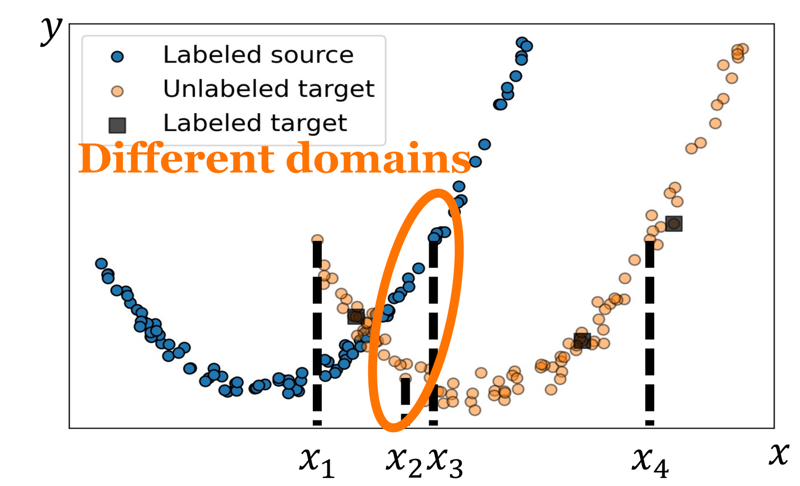
$f(x_2) \approx f(x_3)$ if $x_2 \approx x_3$ (Homogeneous Case)

➢ x_2 and x_3 from source domain



$y_2 \neq y_3$ if $x_2 \approx x_3$ (Heterogeneous Case)

➢ x_2 from target domain
➢ x_3 from source domain



❑ Definition

DINO: $$\tilde{f}(x, \mathbb{P}) \coloneqq f_\theta(x) \cdot g_{w_g}(\mathbb{P}|x) = \left(\phi_{\theta^{<L}}(x)^T w\right) \cdot \left(\Phi_x(\mathbb{P})^T w_g\right) = w^T\left(\phi_{\theta^{<L}}(x)\Phi_x(\mathbb{P})^T\right) w_g$$

Input representation learning

A fully-connected NN: $f_\theta(x) = \phi_{\theta^{<L}}(x)^T w$

($\theta^{<L}$: Parameters of the first $L-1$ layers; w: Parameters of the output layer)

Input-oriented distribution representation learning

Infinitely-wide $f_\theta(\cdot)$ ➡ NNGP kernel space K_X

➡ $\Phi_x(\mathbb{P}) = \sum_{i=1}^{n} \beta_{x,\tilde{x}_i} \langle \cdot, \tilde{x}_i \rangle_{K_X}$ ➡ $g_{w_g}(\mathbb{P}|x) = \Phi_x(\mathbb{P})^T w_g$

Algorithms

❑ DINO-INIT

➢ At initialization, DINO is a Gaussian process with adaptive NNGP kernel

Under random initialization, we have $\tilde{f}(\cdot) \sim \mathcal{N}(0, K^{DA})$ with

$$K^{DA}\left((x,\mathbb{P}),(x',\mathbb{P}')\right) = K_X(x,x') \cdot K_{\mathcal{P}|X}(\mathbb{P},\mathbb{P}'|x,x')$$

where $K_X(\cdot,\cdot)$ is the NNGP kernel, and $K_{\mathcal{P}|X}(\cdot,\cdot)$ is a distribution kernel, i.e.,

$$K_{\mathcal{P}|X}(\mathbb{P},\mathbb{P}'|x,x') = \sum_{i=1}^{n}\sum_{j=1}^{n'} \beta_{x,\tilde{x}_i}\beta_{x',\tilde{x}_j} K_X(\tilde{x}_i,\tilde{x}_j)$$

➢ Adaptive Gaussian process
- Prior GP $\tilde{f}(\cdot) \sim \mathcal{N}(0, K^{DA})$
- Prediction function $p(Y|X_*^{tgt}) = \mathcal{N}(\bar{\mu}, \bar{\Sigma})$

$$\bar{\mu} = K^{DA}(X_*^{tgt}, X)C^{-1}Y \qquad \bar{\Sigma} = K^{DA}(X_*^{tgt}, X_*^{tgt}) - K^{DA}(X_*^{tgt}, X)C^{-1}K^{DA}(X_*^{tgt}, X)^T$$

❑ DINO-TRAIN

➢ Gradient descent training with the following objective function

$$\mathcal{L}(\theta) = \underbrace{\frac{\alpha}{2n_{src}}\sum_{i=1}^{n_{src}}\left(\tilde{f}(x_i^{src},\mathbb{P}^{src}) - y_i^{src}\right)^2 + \frac{1-\alpha}{2n_{tgt}^l}\sum_{j=1}^{n_{tgt}^l}\left(\tilde{f}(x_j^{tgt},\mathbb{P}^{tgt}) - y_j^{tgt}\right)^2}_{\text{Supervised loss over labeled examples}} + \underbrace{\frac{\mu}{2}\mathrm{MMD}^2_{\Theta_{DA}}(\mathbb{P}^{src},\mathbb{P}^{tgt})}_{\text{Empirical MMD-NTK}}$$

➢ Empirical Maximum Mean Discrepancy (MMD) over training dynamics

$$\mathrm{MMD}^2_{\Theta_{DA}}(\mathbb{P}^{src},\mathbb{P}^{tgt}) = \left\| \frac{1}{n_{src}}\sum_{i=1}^{n_{src}} \nabla_\theta \tilde{f}(x_i^{src},\mathbb{P}^{src}) - \frac{1}{n_{tgt}}\sum_{j=1}^{n_{tgt}} \nabla_\theta \tilde{f}(x_j^{tgt},\mathbb{P}^{tgt}) \right\|^2_{\mathcal{H}_{DA}}$$

Experiments

Methods	RL → RC	RL → T	RC → RL	RC → T	T → RL	T → RC	Avg.
NNGP [34]	$0.313_{\pm 0.001}$	$0.438_{\pm 0.004}$	$0.356_{\pm 0.005}$	$0.515_{\pm 0.008}$	$0.367_{\pm 0.001}$	$0.324_{\pm 0.004}$	0.386
NTKGP [25]	$0.396_{\pm 0.001}$	$0.365_{\pm 0.001}$	$0.200_{\pm 0.007}$	$0.390_{\pm 0.003}$	$0.390_{\pm 0.000}$	$0.354_{\pm 0.003}$	0.349
AT-GP [7]	$0.214_{\pm 0.011}$	$0.209_{\pm 0.002}$	$0.227_{\pm 0.010}$	$0.198_{\pm 0.002}$	$0.236_{\pm 0.000}$	$0.249_{\pm 0.000}$	0.222
TL-NTK [38]	$0.206_{\pm 0.004}$	$0.200_{\pm 0.002}$	$0.213_{\pm 0.000}$	$0.197_{\pm 0.000}$	$0.226_{\pm 0.001}$	$0.218_{\pm 0.000}$	0.210
DINO-INIT (ours)	$0.204_{\pm 0.001}$	**$0.185_{\pm 0.006}$**	**$0.207_{\pm 0.003}$**	**$0.182_{\pm 0.004}$**	**$0.218_{\pm 0.001}$**	**$0.212_{\pm 0.001}$**	**0.201**
DINO-TRAIN (ours)	**$0.193_{\pm 0.001}$**	$0.194_{\pm 0.003}$	**$0.207_{\pm 0.003}$**	$0.188_{\pm 0.002}$	$0.226_{\pm 0.001}$	$0.218_{\pm 0.001}$	0.204

Results on dSprites

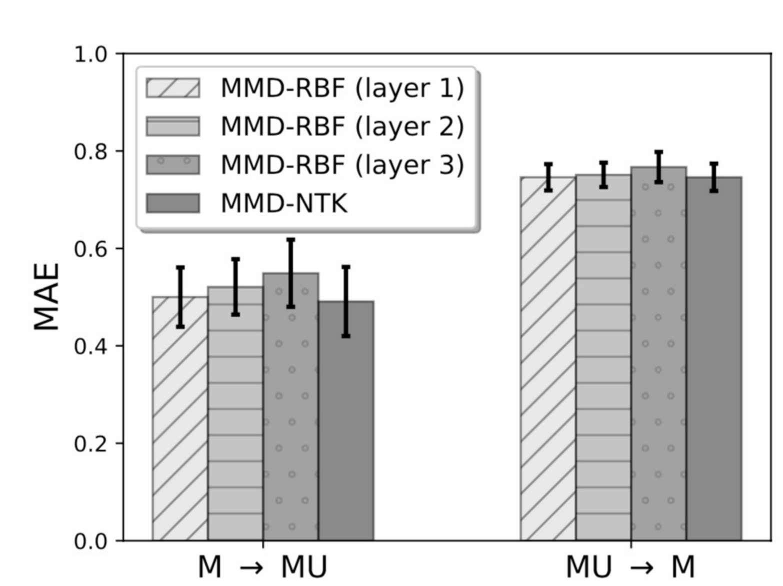
Methods	C → N	C → S	N → C	N → S	S → C	S → N	Avg.
NNGP [34]	$2.041_{\pm 0.001}$	$1.823_{\pm 0.001}$	$0.445_{\pm 0.002}$	$0.624_{\pm 0.001}$	$0.197_{\pm 0.002}$	$0.459_{\pm 0.002}$	0.932
NTKGP [25]	$1.345_{\pm 0.002}$	$1.227_{\pm 0.000}$	$0.323_{\pm 0.002}$	$0.529_{\pm 0.004}$	$0.248_{\pm 0.001}$	$0.425_{\pm 0.002}$	0.683
AT-GP [7]	$0.194_{\pm 0.005}$	$0.259_{\pm 0.002}$	**$0.104_{\pm 0.001}$**	$0.252_{\pm 0.005}$	$0.118_{\pm 0.003}$	$0.189_{\pm 0.006}$	0.186
TL-NTK [38]	$0.164_{\pm 0.001}$	**$0.231_{\pm 0.000}$**	$0.124_{\pm 0.005}$	$0.242_{\pm 0.002}$	$0.125_{\pm 0.001}$	$0.197_{\pm 0.004}$	0.181
DINO-INIT (ours)	$0.128_{\pm 0.001}$	$0.233_{\pm 0.003}$	$0.114_{\pm 0.002}$	**$0.227_{\pm 0.002}$**	**$0.112_{\pm 0.001}$**	**$0.181_{\pm 0.005}$**	**0.166**
DINO-TRAIN (ours)	**$0.127_{\pm 0.002}$**	$0.240_{\pm 0.003}$	$0.127_{\pm 0.000}$	$0.243_{\pm 0.000}$	$0.128_{\pm 0.001}$	$0.194_{\pm 0.001}$	0.177

Results on MPI3D

Lower is better

Methods	M → MU	MU → M
NNGP [34]	$0.562_{\pm 0.001}$	$0.672_{\pm 0.010}$
NTKGP [25]	$0.562_{\pm 0.004}$	$0.702_{\pm 0.010}$
AT-GP [7]	**$0.308_{\pm 0.006}$**	$0.593_{\pm 0.025}$
TL-NTK [38]	$0.316_{\pm 0.008}$	$0.488_{\pm 0.027}$
DINO-INIT (ours)	$0.316_{\pm 0.007}$	$0.645_{\pm 0.017}$
DINO-TRAIN (ours)	$0.314_{\pm 0.009}$	**$0.443_{\pm 0.030}$**

Results on Plant Phenotyping



Conclusion

❑ **Problem**: We study the domain adaptation regression problem in term of convergence and generalization when using deep neural networks.
❑ **Algorithm**: Distribution-informed neural network (DINO) is proposed for learning domain heterogeneity, followed by two instantiated algorithms based on random initialization and gradient descent training.
❑ **Evaluation**: The efficacy of the proposed algorithms is verified on several domain adaptation regression tasks.

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