Cross-Modal Fine-Tuning Align then Refine

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AI lab tranning

2024/05/29

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- 1 Introduction
- Implement ORCA

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Introduction

Transfer learning:

- Reuse of a pre-trained model on a new problem.
- Models can apply what they have learned from large amounts of unlabeled data to downstream tasks.

Existing research:

focuses on in-modality transfer within these well-studied areas.

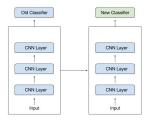


Figure 1: The early and middle layers are used and we only retrain the latter layers

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Cross-Modal Fine-Tuning

Problem: Could cross-modal fine-tuning have immense impact on less-studied areas?

 could we use pretrained BERT models to tackle genomics tasks, or vision transformers to solve PDEs?

ORCA:

- cross-modal fine-tuning workflow.
- prevent the distortion of the pretrained weights.
- exploit the knowledge encoded in the pretrained model.

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- 2 ORCA
- Implement ORCA

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ORCA work flow

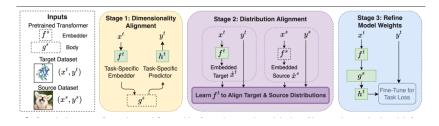


Figure 2: ORCA's three-stage fine-tuning workflow

ORCA:

- Dimensionality Alignment:
 - generate task-specific embedder and predictor.
- Distribution Alignment:
 - train the the embedding network.
- **Refine model weight**: fine-tuning to minimize the target loss.

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Problem setup

Denote:

- A domain \mathcal{D} consists of a feature space \mathcal{X} , a label space \mathcal{Y} , and a joint probability distribution $P(\mathcal{X}, \mathcal{Y})$.
- The target domain \mathcal{D}^t and source (pretraining) domain \mathcal{D}^s
- $\mathcal{X}^t \neq \mathcal{X}^s$, $\mathcal{Y}^t \neq \mathcal{Y}^s$, and $P_t(\mathcal{X}^t, \mathcal{Y}^t) \neq P_s(\mathcal{X}^s, \mathcal{Y}^s)$
- embedder *f* that transforms input *x* into a **sequence of features**.
- model body g that applies a series of pretrained attention layers to the embedded features.
- predictor h that generates the outputs with the desired shape.

Goal:

- Given target data $\{(x_{t_i}, y_{t_i})\}_{i=1}^n$ sampled from a joint distribution P^t in domain \mathcal{D}^t ,
- learn a model m^t that correctly maps each input x^t to its label y^t

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Dimensionality Alignment

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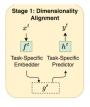


Figure 3: Dimensionality Alignment

Goal: addressing the problem of dimensionality mismatch. **Custom Embedding Network**:

- The target embedder $f^t: \mathcal{X} \to \dot{\mathcal{X}}$ with $\dot{\mathcal{X}}$ is feature space.
- f^t is composed of a convolutional layer.

Custom Prediction Head

• The prediction head h^t take $\dot{y} \in \dot{\mathcal{Y}}$ as input and return a task-dependent output tensor.

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Distribution Alignment

Goal: manipulate the target data so that they become closer to the pretraining modality.

- train the embedder before actually fine-tuning the model body.
- makes the embedded target features resemble the source features.
- key idea.

Denote:

- $f^s: \mathcal{X}^s \to \dot{\mathcal{X}}$ is the pretrained source embedder.
- We can learn f^t by minimize $D(P(f^t(x^t), y^t)||P(f^s(x^s), y^s))$
- *D* is a metric for measuring distribution distance(MMD, OTDD, Euclidean).

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Implement OTDD for Distribution Alignment

- Compute distance between two dataset : $\mathcal{D}^s = (\dot{x}^s, y^s)$ and $\mathcal{D}^t = (\dot{x}^t, v^t)$
- OTDD represents each class label as a distribution over the in-class features:

$$y \mapsto \alpha_y(X) = P(\dot{X} \mid Y = y)$$

• We can compute distance between feature-label pairs as :

$$d_Z((x,y),(x',y')) = \left[d_{\mathcal{X}}(x,x')^p + W_p^p(\alpha_y,\alpha_{y'})\right]^{\frac{1}{p}}$$

• we can finally use optimal transport to compute OTDD:

$$d_{ ext{OT}}(D^s, D^t) = \min_{\pi \in \Pi(lpha, eta)} \int_{Z imes Z} d_Z(z^s, z^t)^p \ \pi(z^s, z^t)$$

•
$$z = (\dot{x}, y)$$

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Research questions

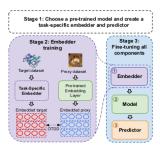


Figure 4: ORCA work flow

- 1 How does the choice of proxy dataset affect performance?
- 2 Does doing (more) embedder training improve performance?
- What do the embedder and the pre-trained model contribute individually?
- 4 How much pre-training is necessary for cross-modal transfer?

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Experimental setup

Transformers pre-train model:

- **1** RoBERTa-base(Liu et al.,2019) for 1*D* tasks.
- 2 Swin-base(Liu et al.,2021) for 2D tasks.

Embedder traing

Using OTDD.

Target dataset

- 1 1D datasets: Satellite, DeepSEA, and ECG
- 2 2D datasets: NinaPro, CIFAR-100, and Darcy Flow.

Proxy datasets

- 1 CIFAR-10 (Krizhevsky, 2009) for all 2D tasks.
- 2 CoNLL 2003 (Tjong Kim Sang and De Meulder, 2003) for all 1D tasks.

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How does the choice of proxy dataset affect performance?

Experiment with the choice of proxy dataset for the tasks.

 Base line: embedder is trained with different proxy datasets or not trained.

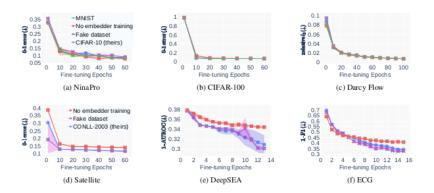


Figure 5: Per-epoch fine-tuning performance

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How does the choice of proxy dataset affect performance?

Paper finding:

 Embedder training does play a role in the 1D tasks, but does not matter for 2D tasks.

Questions:

- 1 Can we trust this conclusion (just comparing 4 dataset)?
- 2 Why are there differences between 2D tasks and 1D tasks?

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Does doing (more) embedder training im- prove performance?

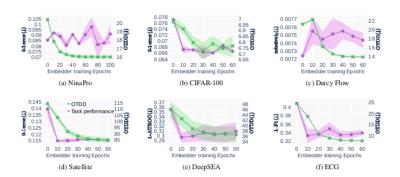


Figure 6: Per-epoch embedder training comparing OTDD

Paper finding:

 Embedder training is unnecessary in 2/6 tasks, training the embedder more can even lead to worse task performance.

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What do the embedder and the pre-trained model contribute individually?

Experiment with freezing different parts of the pipeline:

• Freezing just the embedder, just the model, or both

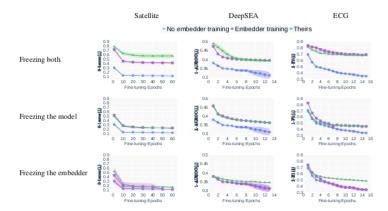


Figure 7: Freezing just the embedder, just the model, or both.

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What do the embedder and the pre-trained model contribute individually?

Paper finding:

- fine-tuning the pre-trained model is a critical component of ORCA.
- while training the embedder is important for ORCA's success on these datasets.
 - it need not be fine-tuned beyond that.

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Pre-training is not always necessary

Use RoBERTa models pre-trained on **different amounts of English data**: 10B,100M, 10M,...

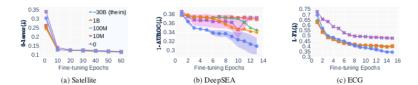


Figure 8: Effect of different amounts of pre-training data on downstream performance.

Paper finding:

 the amount of pre-training has a notice able effect only at certain(30B) scales.

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Conclusion

In 1D task:

- 1 some amount of **embedder training** is **necessary**.
- more embedder training can even hurt performance on the target task.
- 3 using a pre-trained model is actually not necessary.

In 2D task:

1 embedder training does not help at all.

Questions:

- 1 Can we trust this conclusion (just comparing 4 dataset)?
- 2 Why are there differences between 2D tasks and 1D tasks?

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Idea for question about differences between 2D tasks and 1D tasks.

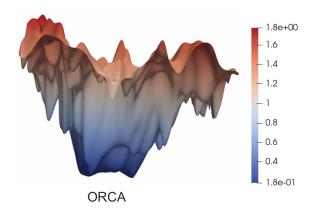


Figure 9: orca loss in Ninapro dataset

ORCA: unstable training, trapped in unfavorable local optima.

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Introduction

ORCA:

- faces instability during training.
- potentially leading to suboptimal results as it is prone to getting trapped in unfavorable local optima.

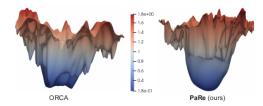


Figure 10: Loss landscape

Patch Replacement(PaRe):

 Motivated by traditional data augmentation techniques like Mixup (Zhang et al., 2017) and CutMix (Yunet al., 2019)

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Patch Replacement(PaRe)

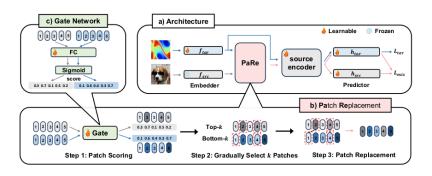


Figure 11: PaRe Overview

Embedder:

- pre-trained embedder $f_s: \mathcal{X}^s \to \tilde{\mathcal{X}}^s$
- target embedder f_t is randomly initialized $f_t: \mathcal{X}^t \to \tilde{\mathcal{X}}^t$

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PaRe

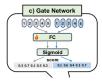


Figure 12: Patch scoring

Patch scoring:

- The source embeddings $\tilde{X}_s \in \mathbb{R}^{N \times D}$ contain N patches, where $\tilde{X}_s = \{\tilde{x}_{s1}, \tilde{x}_{s2}, \dots, \tilde{x}_{sN}\}.$
- Score each patch \tilde{x}_{si} from the source and \tilde{x}_{ti} from the target using a gate network.

$$S_s = \sigma(F_C(\tilde{X}_s))$$

• The higher the score, the more critical information the patch contains

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PaRe

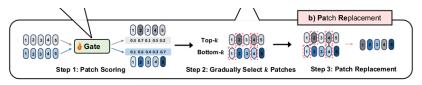


Figure 13: Pa Re

Patches replacement

- keep the positions of the top (N k) target patches with the highest scores fixed.
- replace the bottom (*k*) target patches with the lowest scores with the top (*k*) source patches with the highest scores.
- k linearly decreases with the number of training epochs:

$$k = k_0(1 - \frac{\text{ep}_{\text{current}}}{\text{ep}_{\text{current}}}$$

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Loss function

Denote:

- Output of patchs replacement \tilde{X}^m for source and target.
- Output of source encoder $g(\tilde{X}^m)$.
- source prediction $p^{ms} = h_s\left(g(\tilde{X}^m)\right)$ and target prediction $p^{mt} = h_t\left(g(\tilde{X}^m)\right)$.
- Weight $\lambda = \frac{k}{k_0}$.

Loss function:

• Calculate the mixed loss \mathcal{L}_{mix} using mixed embeddings \tilde{X}^m .

$$\mathcal{L}_{\text{mix}} = (1 - \lambda)\mathcal{L}_{\text{tar}}(p^{mt}, y_t) + \lambda\mathcal{L}_{\text{src}}(p^{ms}, y_s)$$

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Experiment Setup

Pre-train model:

- **1** RoBERTa (Liu et al., 2019) for 1*D* tasks.
- 2 Swin Transformers (Liu et al., 2021) for 2D tasks.

Proxy datasets:

- 1 2D classification tasks: CIFAR10, Tiny-ImageNet.
- 2 D dense prediction tasks: VOC.
- 3 1D tasks: CoNLL-2003.

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Overall results

NAS-Bench-360:

- comprises four 2D classification tasks, three 2D dense prediction tasks, and three 1D tasks.
- PaRe achieves the best performance across all tasks.

	CIFAR-100 0-1 error (%)	Spherical 0-1 error (%)	Darcy Flow relative ℓ_2	PSICOV MAE ₈	Cosmic 1-AUROC	NinaPro 0-1 error (%)	FSD50K 1-mAP	ECG 1-F1 score	Satellite 0-1 error (%)	DeepSEA 1-AUROC
Hand-designed	19.39	67.41	8.00E-03	3.35	0.127	8.73	0.62	0.28	19.80	0.30
NAS-Bench-360	23.39	48.23	2.60E-03	2.94	0.229	7.34	0.60	0.34	12.51	0.32
DASH	24.37	71.28	7.90E-03	3.30	0.190	6.60	0.60	0.32	12.28	0.28
Perceiver IO	70.04	82.57	2.40E-02	8.06	0.485	22.22	0.72	0.66	15.93	0.38
FPT	10.11	76.38	2.10E-02	4.66	0.233	15.69	0.67	0.50	20.83	0.37
NFT	7.67	55.26	7.34E-03	1.92	0.170	8.35	0.63	0.44	13.86	0.51
ORCA	6.53	29.85	7.28E-03	1.91	0.152	7.54	0.56	0.28	11.59	0.29
PaRe	6.25	25.55	7.00E-03	0.99	0.121	6.53	0.55	0.28	11.18	0.28

Figure 14: Prediction errors (↓) across 10 diverse tasks on NAS-Bench-360.

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Overall results(.cnt)

PDEBench:

• comprises multiple scientific ML-related datasets, with a focus on the physics domain.

	Advection 1D	Burgers 1D	Diffusion-Reaction 1D	Diffusion-Sorption 1D	Navier-Stokes 1D	Darcy-Flow 2D	Shallow-Water 2D	Diffusion-Reaction 2D
PINN	6.70E-01	3.60E-01	6.00E-03	1.50E-01	7.20E-01	1.80E-01	8.30E-02	8.40E-01
FNO	1.10E-02	3.10E-03	1.40E-03	1.70E-03	6.80E-02	2.20E-01	4.40E-03	1.20E-01
U-Net	1.10E+00	9.90E-01	8.00E-02	2.20E-01	-	-	1.70E-02	1.60E+00
ORCA	9.80E-03	1.20E-02	3.00E-03	1.60E-03	6.20E-02	8.10E-02	6.00E-03	8.20E-01
PaRe	2.70E-03	8.30E-03	2.60E-03	1.60E-03	6.62E-02	8.06E-02	5.70E-03	8.18E-01

Figure 15: Normalized Root Mean Squared Errors (nRMSEs, ↓) across 8 tasks of PDEBench

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Limitation

- Determining the most suitable source modality proxy dataset based on the target modality dataset remains a **challenge**.
- **2** a modality-agnostic data augmentation method is necessary to prevent model overfitting and enhance cross-modal fine- tuning.

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Introduction

The cross-modal transfer is not as straightforward as the in-modality transfer due to two challenges:

- 1 The input and label space are different across modalities.
- The knowledge required for addressing tasks in different modality may also differ.

Key problem:

- What knowledge from source modality is transferred via the pretrained model?
- How does it benefit the target modality?

MoNa: Improves the cross-modal transfer with two-stage training.

- 1 leverages meta learning to learn an optimal target embedder.
- vanilla finetuning.

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Notations

Model Architecture: g_{θ}

- An embedder $e(\cdot; \theta_e)$.
- A transformer encoder $f(\cdot; \theta_f)$.
- A predictor $h(\cdot; \theta_h)$.
- The parameter of full model as $\theta = \{\theta_e, \theta_f, \theta_h\}$.
- Pretrained weights of the source model as $\theta_0^S = \{\theta_{e_0}^S, \theta_{f_0}^S, \theta_{h_0}^S\}$.
- Target model $\theta^T = \{\theta_e^T, \theta_f^T, \theta_h^T\}$.
- Vanilla finetuning :

$$heta_T^* = rg \min_{ heta_T} \sum_{i=1}^{n_T} \ell\left(g_{ heta}^T(x_i^T), y_i^T
ight),$$

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Distortion of learned source modality knowledge

Problem:

• There lacks a general metric measuring the degree of knowledge reuse during transfer.

Expectation:

• Smaller distortion if more source knowledge is reused to solve target task.

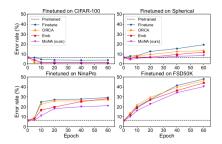


Figure 16: Linear probing results on CIFAR-10.

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Distortion of learned source modality knowledge(.cnt)

Finding:

- More epochs leads to larger distortion of source knowledge on all target modalities except for CIFA-100.
- A large discrepancy may hinder the effectiveness of cross-modal transfer.
- Embedder training:
 - Mitigates the knowledge misalignment between target and source.
 - Reduces the model distortion during its adaptation towards target tasks.
- The key to effective transfer:
 - Learn a target embedding function $e^T: X \to \hat{X}$.
 - makes the target conditional distribution $P(Y^t|\hat{X})$ more aligned with the source knowledge.

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MoNA: Modality Knowledge Alignment

MoNa:

- 1 Stage 1: Target embedder training.
- 2 Stage 2: Full finetuning.

Target embedder training:

• The **inner-loop** is the optimization of the model on target dataset.

$$\theta^{\mathcal{T}^{\star}}(\phi_e) = \arg\min L_{\text{inner}}(x_t, y_t; \phi_e)$$

- Where L_{inner} is the target loss.
- Virtually update model weight : $\theta^{T} = \theta^{T} \alpha \nabla \mathcal{L}_{inner}$
- Outer-loop: find optimal embedder parameters ϕ_e^{\star} .
 - resulting optimal target encoder.
 - generates high quality representations of source data.

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MoNA: Modality Knowledge Alignment(.cnt)

Outer-loop:

- Compute source features $\{f_i^S = f(e(x_i^s, \theta_e^s), \theta_f^T)\}$
- Measures the source discriminability of the induced encoder:

$$\begin{aligned} \mathcal{L}_{\text{outer}} &= \mathcal{L}_{\text{align}} + \mathcal{L}_{\text{uniform}} \\ &= -\mathbb{E}_{i,j:y_i = y_j} \left[\left\| f_i - f_j \right\|_2^2 \right] - \log \mathbb{E}_{i,j} \left[e^{-2 \left\| f_i - f_j \right\|_2^2} \right] \end{aligned}$$

• To prevent the embedder from overly focusing on source modality, we have :

$$\mathcal{L}'_{outer} = \lambda \mathcal{L}_{outer} + \mathcal{L}_{inner}$$

• Update the target embedder as :

$$\phi_e = \phi_e - \beta \nabla \mathcal{L}'_{\text{outer}}$$

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MoNA: Modality Knowledge Alignment(.cnt)

Algorithm 1 MoNA: Modality Knowledge Alignment

Input: Source pretrained model $g_{\theta_0^S}$; Learning rate α, β ; Maximum iterations I_1, I_2 .

Output: Model for the target task: $g_{\theta^{\tau}}$.

Stage 1: Target embedder training

for $iter = 1, 2, \cdots, I_1$ do

Initialize the target model $g_{\theta^{T}}$ with ϕ_{e} and $\theta_{f_{0}}^{S}$.

Virtually update: $\boldsymbol{\theta}^{\mathcal{T}^*} = \boldsymbol{\theta}^{\mathcal{T}} - \alpha \nabla_{\boldsymbol{\theta}^{\mathcal{T}}} \mathcal{L}_{inner}$.

Compute source features $\{ oldsymbol{f}_i^s \}$ with $oldsymbol{ heta}_{e_0}^{\mathcal{S}}$ and $oldsymbol{ heta}_f^{\mathcal{T}^*}$.

Obtain outer-loop loss using Eq. (4).

Update target embedder: $\phi_e \leftarrow \phi_e - \beta \nabla_{\phi_e} \mathcal{L}'_{outer}$.

end for

Stage 2: Full finetuning

for $iter = 1, 2, \cdots, I_2$ do

Initialize the target model $g_{\theta}\tau$ with ϕ_e and $\theta_{f_0}^{\mathcal{S}}$. Update target model towards Eq. (1).

end for

Figure 17: Modality Knowledge Alignment.

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Experiments Setup

Pre-train model:

- **1** RoBERTa (Liu et al., 2019) for 1D tasks.
- 2 Swin Transformers (Liu et al., 2021) for 2D tasks.

Source datasets:

- 1 2D classification tasks: CIFAR10
- **2** 1D tasks : CoNLL-2003.

NAS-Bench-360:

 comprises four 2D classification tasks, three 2D dense prediction tasks, and three 1D tasks.

PDEBench:

• comprises multiple scientific ML-related datasets, with a focus on the physics domain.

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Experiments Result

NAS-Bench-360:

Model	CIFAR-100	Spherical	Darcy Flow	PSICOV	Cosmic	NinaPro	FSD50K	ECG	Satellite	DeepSEA
ORCA	6.53	29.85	7.28 E-3	1.91	0.152	7.54	0.56	0.28	11.59	0.29
MoNA	6.48	27.13	6.80 E-3	0.99	0.121	7.28	0.55	0.27	11.13	0.28
PaRe	6.25	25.55	7.00 E-3	0.99	0.121	6.53	0.55	0.28	11.18	0.28

Table 1: Prediction errors (\downarrow) on ten tasks of NAS-Bench-360.

PDEBench:

Model	Advection	Burgers	Diffusion-Reaction	Diffusion-Sorption	Navier-Stokes	Darcy-Flow	Shallow-Water	Diffusion-Reaction	ı
ORCA	9.80 E-3	1.20 E-2	3.00 E-3	1.60 E-3	6.20 E-2	8.10 E-2	6.00 E-3	8.20 E-1	ı
MoNA	8.8 E-3	1.14 E-2	2.80 E-3	1.60 E-3	5.40 E-2	7.9 E-2	5.70 E-3	8.18 E-1	
PaRe	2.70 E-3	8.30 E-3	2.60 E-3	1.60E-3	6.62 E-2	8.06 E-2	5.70 E-3	8.18 E-1	

Table 2: Normalized Root Mean Squared Errors (nRMSEs, ↓) across 8 tasks of PDEBench.

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Idea

Problem setup:

- Tranformers pre-train body model g_s in domain D^s .
- Dataset $\{x_i^t, y_i^t\}_{i=1}^N$ in domain D^t .
- Dataset $\{x_i^s, y_i^s\}_{i=1}^N$ in domain D^s



Figure 18: proposed model

embedder: f extract feature from input f(.)

- random init for f_t .
- using pre-train and freezing for f_s

predictor: h generate output h(.).

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Idea(cnt.)

Proposed workflow:

- **1** Stage 1 : Contrastive training for embedder.
- Stage 2 : Patch-replacement fine-tuning.

Stage 1: Contrastive training for embedder.

- 1 Step 1 : Data augmentation.
- 2 Step 2: Training target embedder.

Step 1: Data augmentation.

• Pertubing data T times with multi-scale gaussian noise $\{\sigma_i\}_{i=1}^K$.

$$x_i^t = \sqrt{1 - \sigma^2} x_i^{t-1} + \sigma * \epsilon$$

 $\epsilon \sim \mathcal{N}(0, I)$

• We have Expanded Dataset $\{x_i, y_i\}_{i=1}^M$ with $M = N \times K \times T$

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Step 2 : Contrastive training for target embedder

We have:

- feature $z_i = f(x_i)$ is a embedded vector.
- Similarity between two output:

$$cos(z_i, z_j) = \frac{z_i z_j}{||z_i|| * ||z_j||}$$

- **Objective**: Similarity high in the same label, low in the different label.
- Loss function for label Y:

$$\mathcal{L}_{Y} = -\log \frac{\sum_{j}^{y_{j}=Y} \sum_{i}^{y_{i}=Y} cos(z_{i}, z_{j})}{\sum_{i}^{y_{i}=Y} \sum_{j=1}^{M} \lambda_{i,j} cos(z_{i}, z_{j})}$$

• $\lambda_{i,j} \propto \frac{1}{\text{correlation}(y_i, y_i) + \epsilon}$ and $\lambda_{i,j} = 1$ if $y_i = y_j$.

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Patch-replacement fine-tuning

Stage 2: Patch-replacement fine-tuning.

• Using seft-attention for scoring each feature patch.

Training options:

- Freezing embedder.
- 2 Training embedder.

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MMD

Define: MMD is a distance (difference) between feature means. **Denote**:

- X and $\phi(X) \in \mathcal{F}$ is the a feature map.
- Assuming \mathcal{F} satisfies the necessary conditions:
 - X, Y such that $k(X, Y) = \langle \phi(X), \phi(Y) \rangle_{\mathcal{F}}$

Feature Mean:

• Given $\mathcal{X} \sim P$ we have feature means :

$$\mu_P = \mathbb{E}_{X \sim P}[\phi(X)]$$

Maximum mean discrepancy:

$$MMD(P, Q) = \|\mathbb{E}_{X \sim P}[\phi(X)] - \mathbb{E}_{Y \sim O}[\phi(Y)]\|_{\mathcal{T}} = \|\mu_P - \mu_O\|_{\mathcal{T}}$$

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Optimal transport(OP): Comparing by 'transporting'

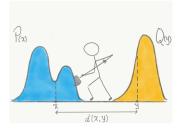


Figure 19: Optimal transport

Optimal transport

- a method to find least-cost schemes to transport dirt and rubble from one place to another.
- $\operatorname{OT}_c(\alpha, \beta) := \min_{\pi \in \Pi(\alpha, \beta)} \int_{Y \vee Y} c(x, y) d\pi(x, y).$
 - $\Pi(\alpha, \beta)$ be the set of joint probability distributions on $X \times X$.
- $W_p(\alpha, \beta) = OT(\alpha, \beta)^{1/p}$ is called the *p*-Wasserstein distance.

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