# Cross-Modal Fine-Tuning

## Align then Refine

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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.

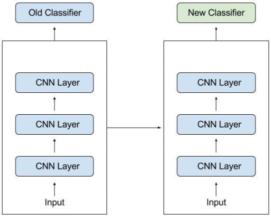



Figure 1: The early and middle layers are used and we only retrain the latter layers

# 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.

# ORCA work flow

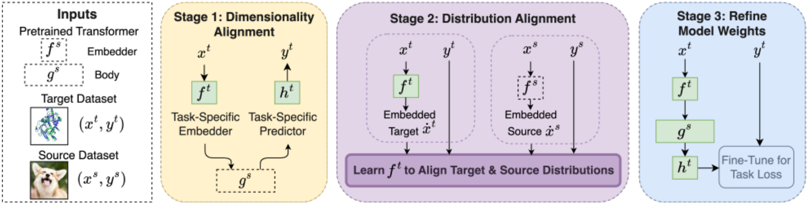



Figure 2: ORCA's three-stage fine-tuning workflow

**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.

# 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 $y^t$

# Dimensionality Alignment

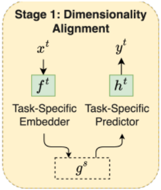



Figure 3: Dimensionality Alignment

**Goal**: addressing the problem of dimensionality mismatch.

**Custom Embedding Network**:

- The target embedder $f^t : \mathcal{X} \rightarrow \dot{\mathcal{X}}$ 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.

# 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**:

- $f^s : \mathcal{X}^s \rightarrow \dot{\mathcal{X}}$ 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).

# Implement OTDD for Distribution Alignment

- Compute distance between two dataset : $\mathcal{D}^s = (\dot{x}^s, y^s)$ and $\mathcal{D}^t = (\dot{x}^t, y^t)$
- 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 :

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

- we can finally use optimal transport to compute OTDD :

$$d_{\mathrm{OT}}(D^s, D^t) = \min_{\pi \in \Pi(\alpha,\beta)} \int_{Z\times Z} d_Z(z^s, z^t)^p \, \pi(z^s, z^t)$$

  - $z = (\dot{x}, y)$

# Research questions

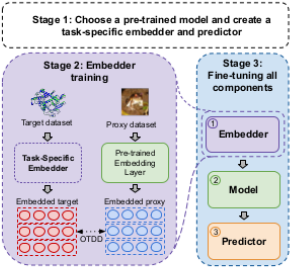



Figure 4: ORCA work flow

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

# 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 2$D$ 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.

# 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**.

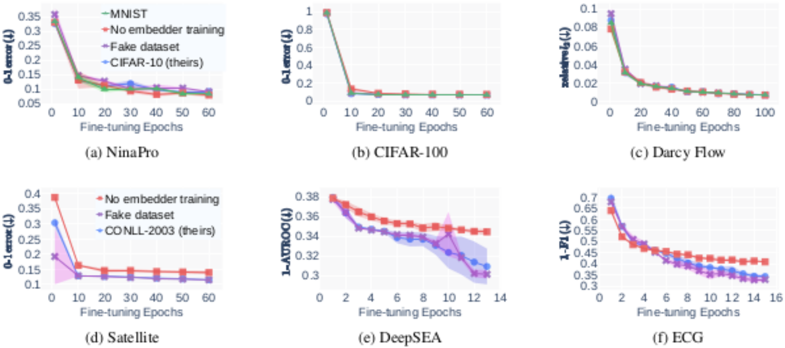



Figure 5: Per-epoch fine-tuning performance

# 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?

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

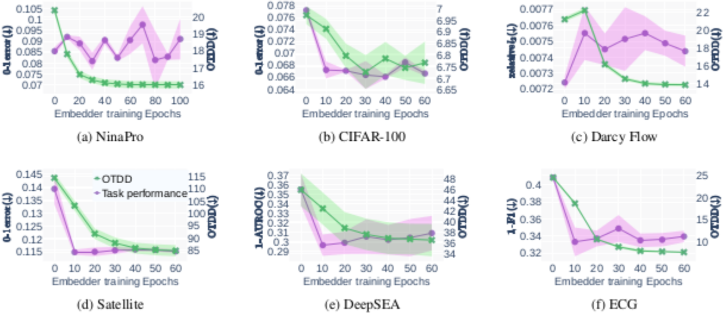



Figure 6: Per-epoch embedder training comparing OTDD

**Paper finding:**

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

# 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

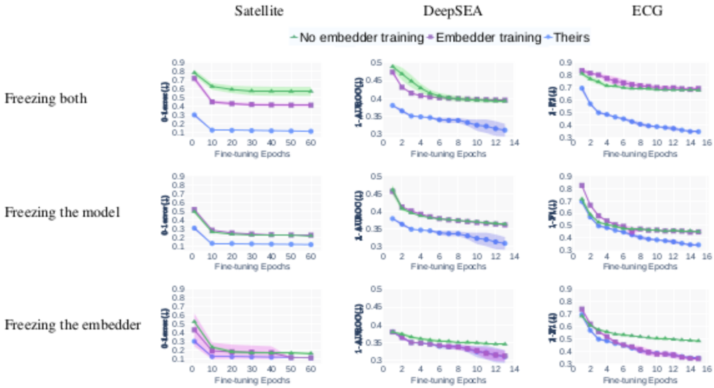



Figure 7: Freezing just the embedder, just the model, or both.

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

**Paper finding:**

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

# Pre-training is not always necessary

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

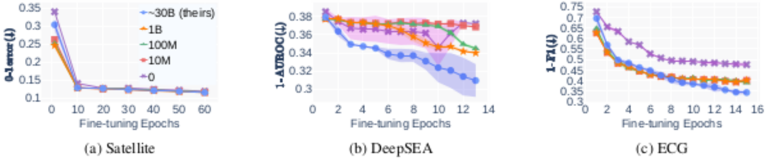



Figure 8: Effect of different amounts of pre-training data on downstream performance.

**Paper finding**:

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

# Conclusion

**In 1D task:**

1. some amount of **embedder training** is necessary.
2. **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?

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

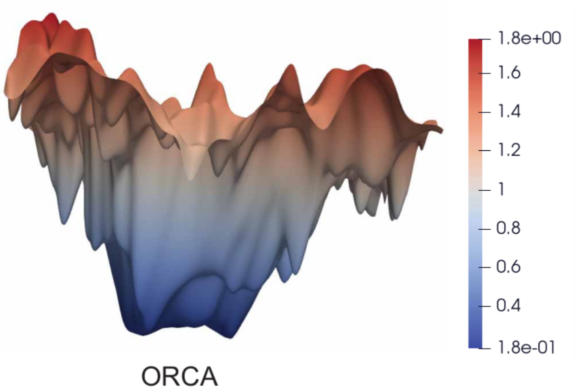



Figure 9: orca loss in Ninapro dataset

**ORCA**: unstable training, trapped in unfavorable local optima.

# Introduction

**ORCA:**

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

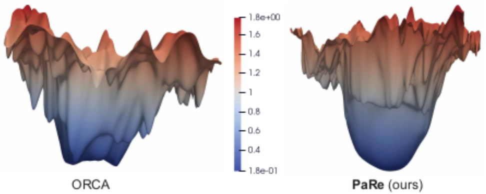



Figure 10: Loss landscape

**Patch Replacement(PaRe):**

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

# Patch Replacement(PaRe)

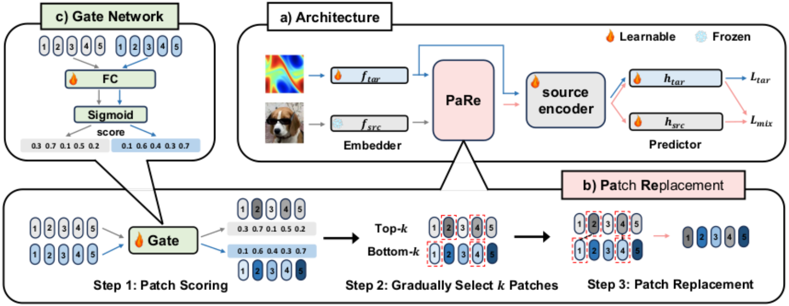



Figure 11: PaRe Overview

## Embedder:

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

# PaRe

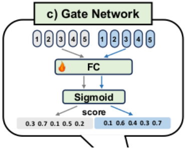



Figure 12: Patch scoring

**Patch scoring:**

- The source embeddings $\tilde{X}_s \in \mathbb{R}^{N \times D}$ contain $N$ patches, where $\tilde{X}_s = \{\tilde{x}_{s1}, \tilde{x}_{s2}, \ldots, \tilde{x}_{sN}\}$.
- 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

# PaRe

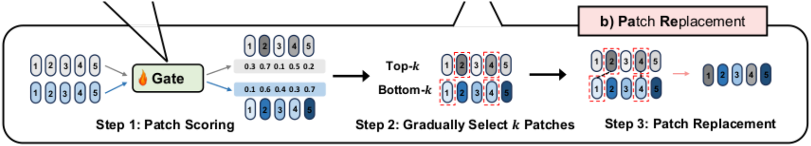



Figure 13: Pa Re

## 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:

$$k = k_0 \left(1 - \frac{\text{ep}_{\text{current}}}{\text{ep}_{\text{total}}}\right)$$

# 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 $\mathcal{L}_{\text{mix}}$ using mixed embeddings $\tilde{X}^m$.

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

# Experiment Setup

**Pre-train model**:

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

**Proxy datasets**:

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

# 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 $\ell_2$ | 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.

# 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

# Limitation

1. 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.

# 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.
2. 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.
2. vanilla finetuning.

# Notations

**Model Architecture**: $g_\theta$

- 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 :

$$\theta_T^* = \arg\min_{\theta_T} \sum_{i=1}^{n_T} \ell\left(g_\theta^T(x_i^T), y_i^T\right),$$

# 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.

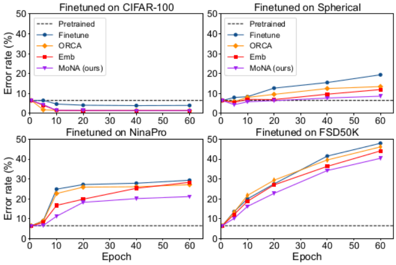



Figure 16: Linear probing results on CIFAR-10.

# 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.

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

# MoNA: Modality Knowledge Alignment(.cnt)

**Outer-loop**:

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

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

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

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

- Update the target embedder as :

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

# MoNA: Modality Knowledge Alignment(.cnt)

**Algorithm 1** MoNA: Modality Knowledge Alignment

**Input:** Source pretrained model $g_{\boldsymbol{\theta}_0^{\mathcal{S}}}$; Learning rate $\alpha$, $\beta$; Maximum iterations $I_1, I_2$.

**Output:** Model for the target task: $g_{\boldsymbol{\theta}^{\mathcal{T}}}$.

**Stage 1: Target embedder training**

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

  Initialize the target model $g_{\boldsymbol{\theta}^{\mathcal{T}}}$ with $\phi_e$ and $\boldsymbol{\theta}_{f_0}^{\mathcal{S}}$.

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

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

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

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

**end for**

**Stage 2: Full finetuning**

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

  Initialize the target model $g_{\boldsymbol{\theta}^{\mathcal{T}}}$ with $\phi_e$ and $\boldsymbol{\theta}_{f_0}^{\mathcal{S}}$.

  Update target model towards Eq. (1).

**end for**

Figure 17: Modality Knowledge Alignment.

# 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.

# 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 (↓) on ten tasks of NAS-Bench-360.

## PDEBench:

| Model | Advection | Burgers | Diffusion-Reaction | Diffusion-Sorption | Navier-Stokes | Darcy-Flow | Shallow-Water | Diffusion-Reaction |
|---|---|---|---|---|---|---|---|---|
| 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 |
| 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.

# Modality semantic knowledge discrepancy

**Denote**:

- Representing the semantic knowledge within a modality using the conditional distribution $P(Y|X)$.

**Problem**: Measure the degree of **"similarity"** of such knowledge between two modalities is challenging.

- Both the data space $\mathcal{X}$ and the label space $\mathcal{Y}$ are different.

**Solution**: Modify the conditional distribution $P(Y^t|X^t)$ and $P(Y^s|X^s)$to make it comparable across modalities.

- Modifying the **input space** : Using embedder.
- Modifying the **label space** is more difficult.

**Assumption**:

- The cardinality of source modality label space is **larger** than the cardinality of the label space of the target modality.

$$|Y^s| \geq |Y^t|$$

# Modality semantic knowledge discrepancy

- Select a subset of the source modality label space $Y_B^s \subseteq Y^s$ such that $|Y_B^s| = |Y^t|$.
- Permutation $\pi(\cdot)$ that adjusts the order of source classes, we have $Y_{\pi,B}^s \hat{=} \pi(Y_B^s)$.

**Definition** : Given the source modality $M^s$ and the target modality $M^t$ satisfying the assumption.

- $\hat{\mathcal{X}}$ is the share input space generated from raw data spaces by embedders.
- $P(Y^s|\hat{X}), P(Y^t|\hat{X})$ are the conditional distribution for the source and target modality.
- The modality semantic knowledge discrepancy between the two modalities is :

$$D(M^s, M^t) = \inf_{\pi,B} d\left(P(Y_{\pi,B}^s \mid \hat{X}), P(Y^t \mid \hat{X})\right)$$

  - $d(\cdot,\cdot)$ is an arbitrary discrepancy measure between two conditional

# Modality semantic knowledge discrepancy

**Problem**: Too much computation cost for finding the optimal permutation $\pi$.

- $|Y^s| = m, |Y^t| = n$ then we conduct random experiment for $C_m^n * n!$ times

**Solution**: Using Approximation Algorithm for Computing Modality Knowledge Discrepancy.

- Source pretrained model $g_{\theta^s}$; Target data $\{x_i^t, y_i^t\}$; $|Y^t| = K$
- Compute the source logit for each target sample: $z_i^s = g_{\theta^s}(x_i^t)$.
- **Randomly select a subset B** of class index from source class.
- Assign the **source category** as $y_{i,B}^S = \arg\max_{k \in B} [z_i^s]_k$.
- **Randomly** shuffle the **index of target labels**: $y^t = \pi(y^t)$.
- We can compute the modality knowledge discrepancy as :

$$D(M^s, M^t) = \frac{1}{n_t} \sum_{i=1}^{n_t} d\left(p(y_B^s \mid x_i^t), p(y^t \mid x_i^t)\right).$$

# Modality semantic knowledge discrepancy

**Algorithm 2** Approximation Algorithm for Modality Knowledge Discrepancy

**Input:** Source pretrained model $g_{\boldsymbol{\theta}_0^s}$; Target data $\{\boldsymbol{x}_i^t, y_i^t\}$; Target task category number $K$; Maximum experiments $I$.
**Output:** Modality Knowledge Discrepancy $D(\mathcal{M}^s, \mathcal{M}^t)$.
Compute the source logit for each target sample: $\boldsymbol{z}_i^s = g_{\boldsymbol{\theta}_0^s}(\boldsymbol{x}_i^t)$.
$min_D \leftarrow 1$.
**for** $exp = 1, 2, \cdots, I$ **do**
    Randomly select a subset $\mathcal{B}$ of class index from source class indexes with the size equals to target class number, $|\mathcal{B}| = K$.
    $y_{i,\mathcal{B}}^s \leftarrow \arg\max_{k \in \mathcal{B}}[\boldsymbol{z}_i^s]_k$
    Randomly shuffle the index of target labels: $y^t \leftarrow \pi(y^t)$, (e.g., $\pi(1) = 2, \pi(2) = 1$.)
    Compute $D_{exp}(\mathcal{M}^s, \mathcal{M}^t)$ using Eq. (11).
    $min_D \leftarrow \min(D_{exp}, min_D)$.
**end for**
Return $min_D$.

Figure 18: Approximation Algorithm for Computing Modality Knowledge Discrepancy

# Introduction

**Partial Differential Equations (PDEs):**

- play a pivotal role in modeling and understanding real-world phenomena.

**Unified PDE Solvers (UPS):**

- Learns unified neural operators for complex time-dependent PDEs.
- Improved efficiency and generalization ability.
- Adapt pretrained Large Language Models (LLMs) to PDE solving.
- Map the current state of a PDE to its future state for general spatiotemporal PDEs.

# Introduction

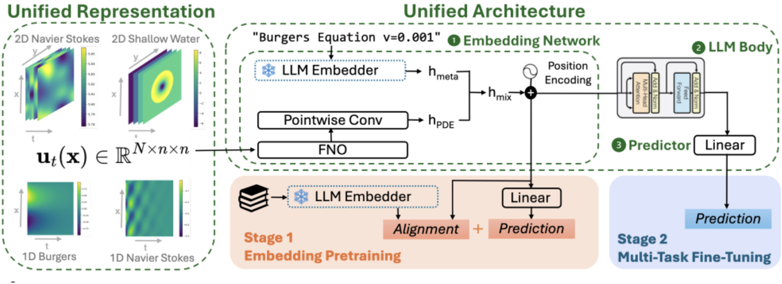



Figure 19: Adapt pretrained LLMs for PDE solving.

**Two key designs:**

1. Unified data representation.
2. Unified network architecture.

# Unified Data Resprentation

**Goal**: Align PDEs with varying dimensions and physical quantities into the same feature space.
Model PDEs that follow the general form:

$$\frac{du(t,x)}{dt} = L\left(u(t,x), \frac{\partial u(t,x)}{\partial x}, \quad \frac{\partial^2 u(t,x)}{\partial x^2}, \cdots\right)$$

$$u(0,x) = u_0(x), \quad B(u(t,y)) = 0$$

- $x \in \Omega \subset \mathbb{R}^d$ is the spatial variable.
- $u : [0,T] \times \Omega \to \mathbb{R}^d$ is a time-varying function defined over the domain $\Omega$ for finite time $T$.
- L is a operator which acts on u and multiple partial derivatives of u w.r.t x.
- $u_0(x) : \Omega \to \mathbb{R}^d$ denotes the PDE's initial condition.
- Operator $B$ defines the boundary condition where $y \in \partial\Omega$ is a point on the domain's boundary.

# Unified Data Resprentation

**Problem Setup**:

- A set of $S$ spatiotemporal PDEs $\{u_s\}_{s=1}^{S}$.
- Each $u^s = \{u_t^s(x)\}_{t=1}^{T_s}$ is a solution to a PDE.
- We have an $n$-point discretization of the functions $\{u_t^s\}_{t=1}^{T}$ at points $W_n^s = \{x_1^s, x_2^s, \ldots, x_n^s\}$, where each $x_i^s \in \mathbb{R}^{d^s}$.

**Unifying Dimension**:

- Let $d = \max_{s \in S} d^s$. We want to represent all datasets in $\mathbb{R}^d$.
- For PDEs with $d_s < d$, the final $d - d_s$ coordinates of $x_i^s \in W_n^s$ are set to zero.

**Unifying Physical Quantities**:

# 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 $D^s$

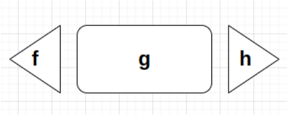



Figure 20: proposed model

**embedder**: $f$ extract feature from input $f(.)$

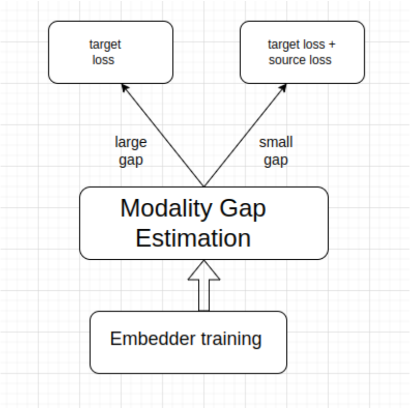
- random init for $f_t$.
- using pre-train and freezing for $f_s$

**predictor**: $h$ generate output $h(.)$.

# Idea(cnt.)

**Proposed workflow:**

1. Stage 1 : Embedder training: mitigate modality gap.
2. Stage 2 : Modality gap estimation.
3. Stage 3 : Full fine-tuning.



# Stage 1: Embedder training

**Goal**: Reduces the model distortion during its adaptation towards target tasks.

**Base line**:

- **Emb** : updates the target embedder using the same task loss as vanilla finetun- ing while keeping the rest of the network frozen.
- **OCRA** : Train embedder by optimizing OTDD distance between source and target.
- **MoNa** : Using **meta-learning** to train embedder.

# Modality gap estimation

**OTDD** :

- Using when label space is discrete.
- Extract feature for target and source: $e_i^t = g^s(f^t(x_i^t))$ and $e_i^s = g^s(f^s(x_i^s))$.
- Measure distance between $\{e_i^t, y_i^t\}_{i=1}^N$ and $\{e_i^s, y_i^s\}_{i=1}^N$.

**MMD** :

- Using when label space is continuous.

**We have** :

- Modality gap $D = D(\mathcal{M}^t, \mathcal{M}^s)$.
- $D > \Gamma$ : modality gap is large. Large distortion of learn source modality knowledge.
  - focus on target loss.

# Full fine-tuning

**Option 1:**

- If modality gap is large : $\mathcal{L} = \mathcal{L}_{\text{target}}$.
- If modality gap is small : $\mathcal{L} = \alpha\mathcal{L}_{\text{target}} + \beta\mathcal{L}_{\text{source}}$

**Option 2:**

- Loss function as: $\mathcal{L} = \alpha\mathcal{L}_{\text{target}} + \frac{\beta}{\epsilon+D}(1 - \frac{ep_{\text{current}}}{ep_{\text{total}}})\mathcal{L}_{\text{source}}$.

# 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**:

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

# Optimal transport(OP): Comparing by 'transporting'


Figure 22: Optimal transport

## Optimal transport

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

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