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AGRIAL

Sim-to-Real Transfer with Asymmetric Temporal Supervision

Using Alignment techniques on an Implicit Neural Representation (INR) based architecture

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PLAN

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2. Task Formulation
3. Lessons From Unsupervised Domain Alignment
4. Modulated Implicit Neural Representations
5. Domain Alignment on an INR-FiLM architecture
6. Use Case
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A Reminder on Transfer Learning

Domain and Task

An arbitrary **domain** is defined by a **feature space** $\mathcal{X}$ and a **marginal distribution** $P(X)$.

$$\mathcal{A} = \{\mathcal{X}, P(X)\}$$

An arbitrary **task** is defined by a **label space** $\mathcal{Y}$ and a **conditional distribution** $P(Y \mid X)$, induced by an unknown predictive function $f(X) = Y$

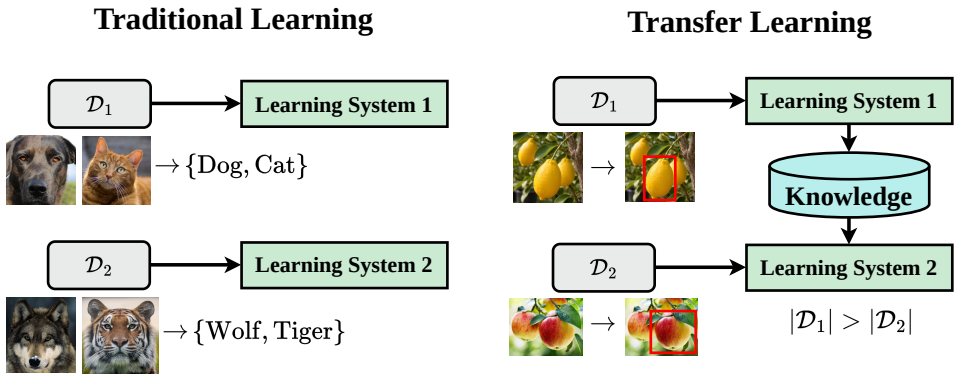
$$\mathcal{T}_{\mathcal{A}} = \{\mathcal{Y}, f\}$$

A domain and its associated task induce a dataset

$$\mathcal{D}_{\mathcal{A}} = \{(X^{(i)}, Y^{(i)})\}_{i=1}^{N}$$

X and Y are random variables, so that $X \in \mathcal{X}$ and $Y \in \mathcal{Y}$

The Classical Transfer Learning Framework



Pan and Yang 2010

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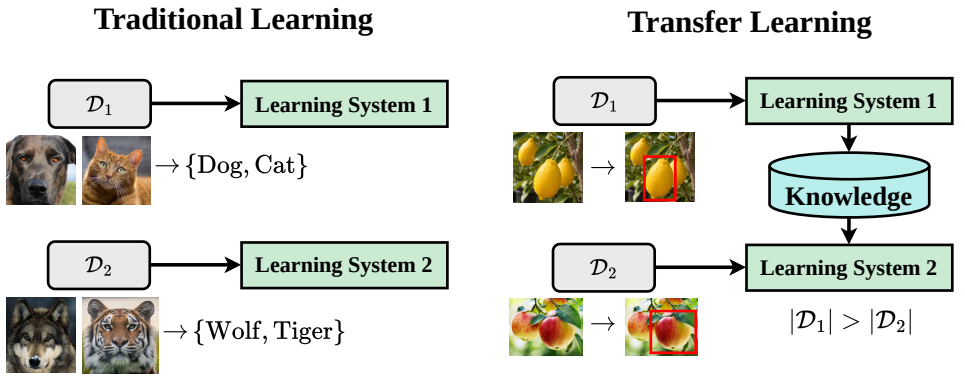

Covariate shift ($P_{\mathcal{S}}(X) \neq P_{\mathcal{R}}(X)$)

Label shift ($P_{\mathcal{S}}(Y) \neq P_{\mathcal{R}}(Y)$)

Concept shift ($P_{\mathcal{S}}(Y \mid X) \neq P_{\mathcal{R}}(Y \mid X)$)

Pan and Yang 2010

Foundations Models: Is **Transfer Learning** a **solved** problem?

What **model of the world** do they have?

Antoine Cornuéjols

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The Classical Paradigm (Pre-2020)

- Neural networks learn **hierarchical representations**
- Each new domain or task requires retraining

Transfer Learning in the Era of Foundation Models

The Classical Paradigm (Pre-2020)

- Neural networks learn **hierarchical representations**
- Each new domain or task requires retraining

Foundation Models (Post-2020)

- FMs learn **universal representations** from massive unlabeled datasets
- Zero-shot capacities
- Each new domain requires **no retraining**, only lightweight adaptation

However...

- Many domains suffer from data scarcity: medical imaging, materials science, industrial fault diagnosis, ...
- Foundation Models learn statistical correlations at scale but have no mechanism to encode causal structure, physical laws, or hard constraints
- Adapation requires dense supervision in the target domain, making low-label regimes out of scope

Task Formulation

- We denote $X \in \mathcal{X}$ as $\mathbf{x} = \{\mathbf{x}^{(d)} \cup \mathbf{x}^{(s)}\}$
- The label $Y \in \mathcal{Y}$ is a time series $\{y_\tau\}_{\tau=0}^{T}$

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In the simulated domain $\mathcal{S}$

$$\theta^* = \arg\min_{\theta} \; \mathbb{E}_{P_{\mathcal{S}}} \left[\sum_{t=0}^{T} \ell(\hat{y}_\tau, \, y_\tau) \right]$$

$$\mathcal{L}_{\mathcal{S}}(\theta) = \frac{1}{N_{\mathcal{S}}} \sum_{i=1}^{N_{\mathcal{S}}} \sum_{\tau=0}^{T} \ell\big(\hat{y}_\tau^{(i)}, \, y_\tau^{(i)}\big)$$

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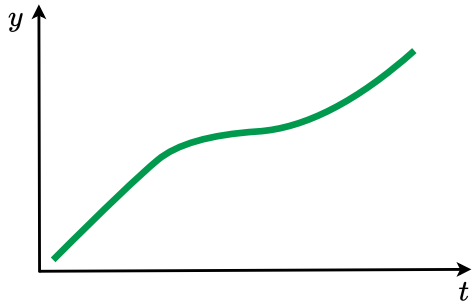
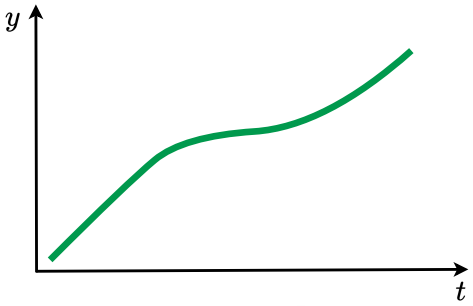


A sample from $D_{\mathcal{S}}$

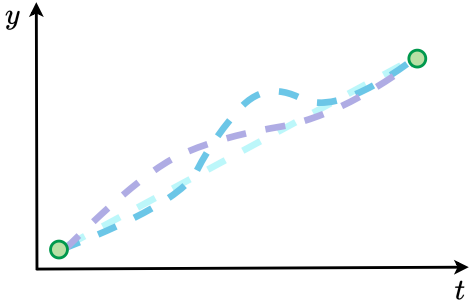
A sample from $D_{\mathcal{R}}$

Available y_t for supervision

Transfer Learning for Time Series with Asymmetric Supervision



A sample from $D_{\mathcal{S}}$

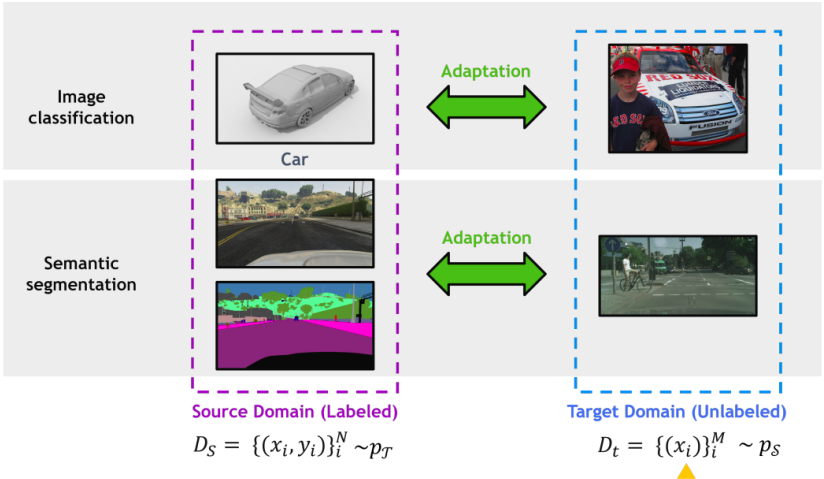


A sample from $D_{\mathcal{R}}$

Available y_t for supervision

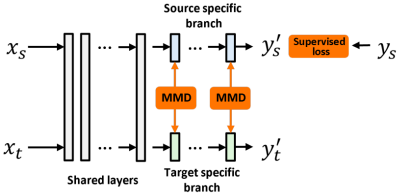
Lessons From Unsupervised Domain Alignment

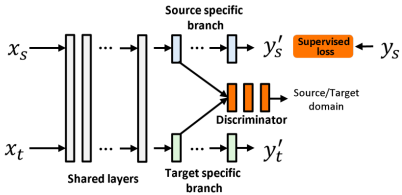
Unsupervised Domain Adaptation



Liu et al. 2022

Unsupervised Domain Adaptation





$$\mathcal{L}_{\text{MMD}} = \mathbb{E}_{x,x'}[k(x,x')] + \mathbb{E}_{y,y'}[k(y,y')] - 2\,\mathbb{E}_{x,y}[k(x,y)],$$

where $x, x' \sim z_{\text{synth}}$, $y, y' \sim z_{\text{real}}$, and the kernel function is $k(x,y) = \exp\left(-\frac{\|x-y\|^2}{2\sigma^2}\right)$

$$\mathcal{L}_{\text{adv}} = -\sum_i \left[y_i \log \sigma(f_i) + (1-y_i) \log\left(1-\sigma(f_i)\right) \right],$$

where $y_i = 0$ denotes source samples, $y_i = 1$ denotes target samples, f_i is the discriminator logit, and $\sigma(\cdot)$ is the sigmoid function.

Liu et al. 2022

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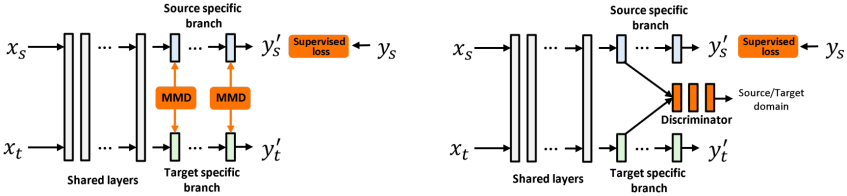

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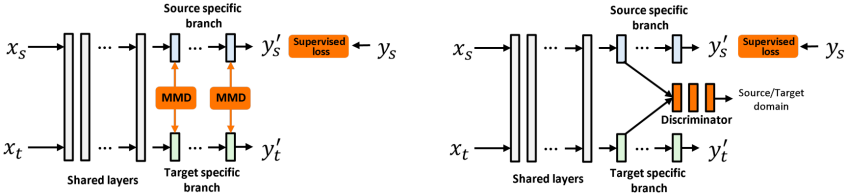

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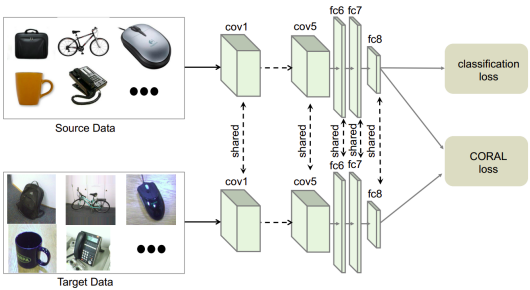
Liu et al. 2022

Unsupervised Domain Adaptation: CORAL



$$\mathcal{L}_{\text{CORAL}} = \frac{1}{4d^2} \|C_s - C_r\|_F^2$$

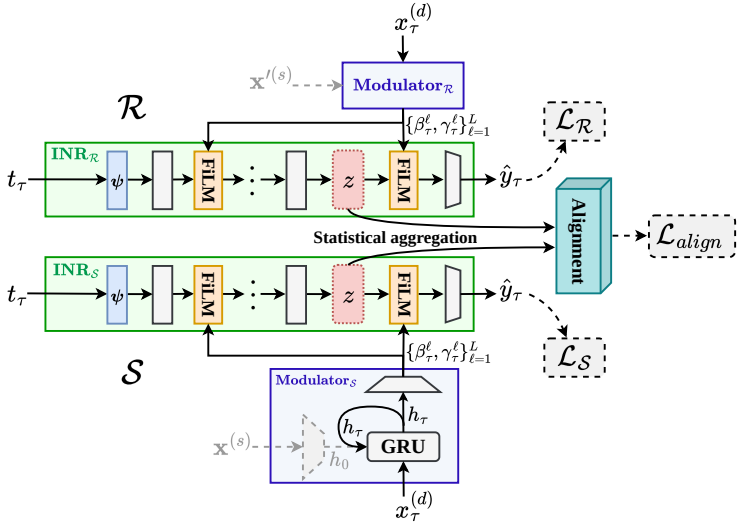
where $C_s, C_r \in \mathbb{R}^{d \times d}$ are the unbiased sample covariance matrices computed from the latent representations, and $\| \cdot \|_F$ denotes the Frobenius norm.

Sun and Saenko 2016

Unsupervised Domain Adaptation

- **Kernel-Based Distribution Matching (MMD):** aligns domain distributions in a Reproducing Kernel Hilbert Space (RKHS).
- **Adversarial Feature Alignment** aligns distributions implicitly via a minimax game between feature extractor and domain discriminator.
- **Alignment via Second-Order Statistics (CORAL)** Minimizes domain shift by matching covariance matrices.

The Proposed Architecture



Modulated Implicit Neural Representations

Implicit Neural Representations (INRs)

Implicit Neural Representations consider the problem of finding a **continuous representation of data**

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Multi Layer Perceptron **(MLPs)** $\rightarrow$ Continuous and fully differentiable.

INR

- Coordinate based MLPs
- Arbitrary resolution at inference
- Memory efficient

Explicit representations

- Point clouds, voxel grids, meshes, ...
- Resolution is fixed at acquisition time
- Less compact representations

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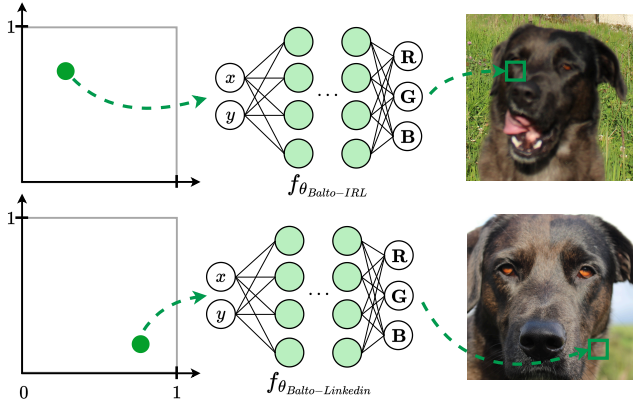
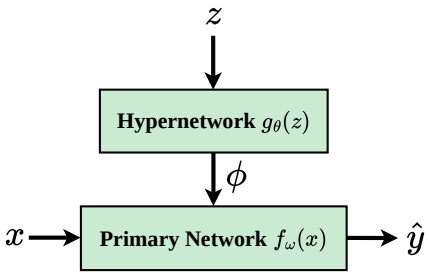
A major problem is spectral Bias!
Positional encoding or **adaptive activation functions** can capture a wide range of frequencies.

INRs for Learning Images Representations

Our function of interest could be simply an image, mapping the coordinates $[x, y]$ to their pixel values $[\mathbf{R}, \mathbf{G}, \mathbf{B}]$.

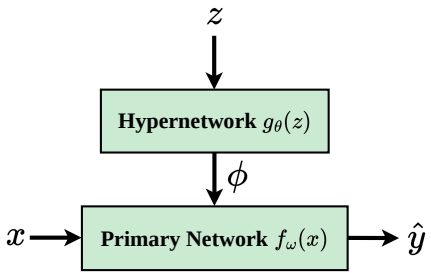


Hypernetworks and Feature-Wise Linear Modulation



$\phi \subseteq \omega$

Hypernetworks and Feature-Wise Linear Modulation



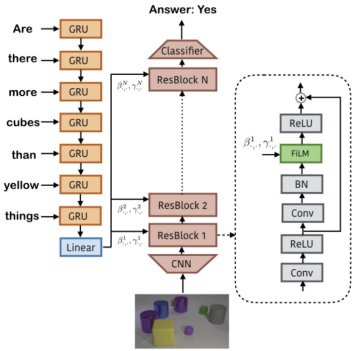
- ✔ A single hypernetwork can parameterize a family of primary networks
- ✔ High expressivity $\rightarrow$ Interesting for Multi-Task Learning
- ✖ Unstable and difficult to train
- ✖ Too expressive for most cases

Ha, Dai, and Le 2016

Hypernetworks and Feature-Wise Linear Modulation

Feature-wise Linear Modulation (FiLM) is a method for conditioning models by inserting feature-wise transformation layers into the primary network.

$$\mathrm{FiLM}(\mathbf{x}) = \gamma(z) \odot x + \beta(z)$$



- ✔ The FiLM generator (**modulator**) is an specialized Hypernetwork
- ✔ Sufficiently complex for most tasks
- ✔ Natural factorization of shared structure from instance-specific variation

Useful for conditioning generative models, performing style transfer, . . .

Perez et al. 2017

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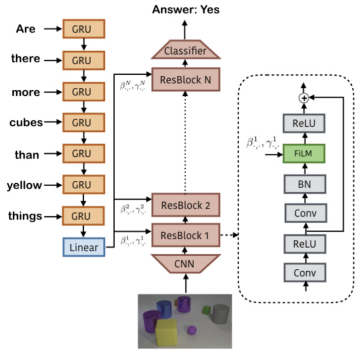

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- ✔ Natural factorization of shared structure from instance-specific variation **(nice for INRs ?)**

Useful for conditioning generative models, performing style transfer, . . .

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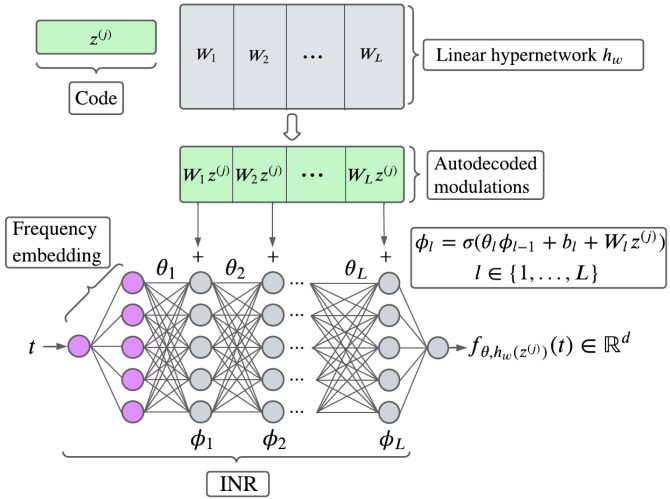
Modulated INRs for Time Series Modeling



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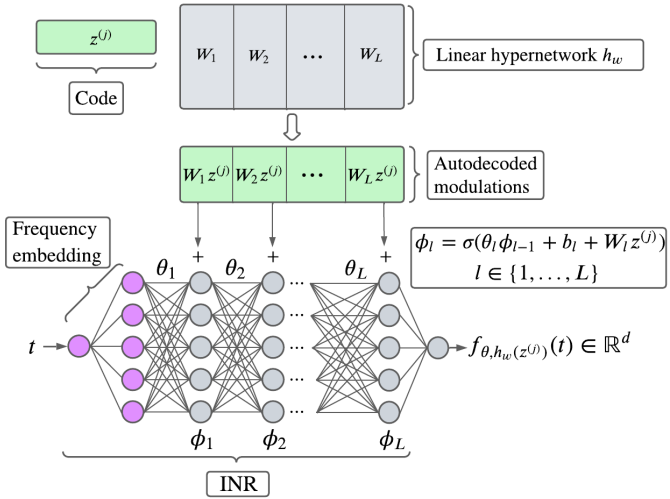

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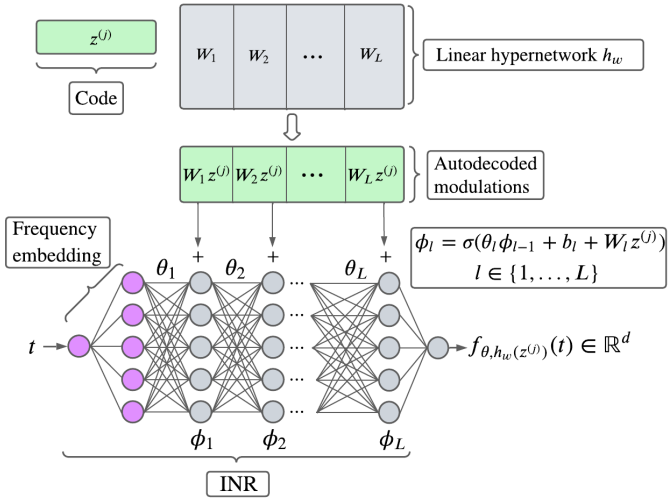

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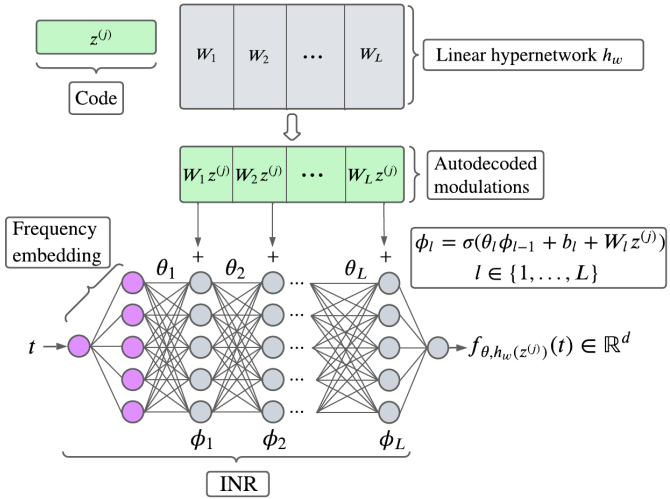

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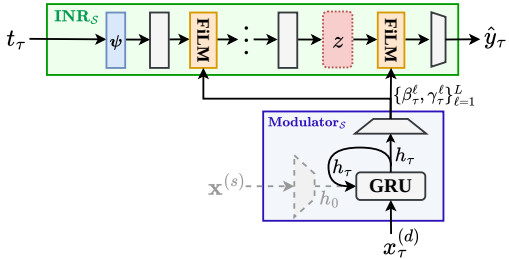
A beautiful example of using INRs for tasks other than representation

Naour et al. 2024

Domain Alignment on an INR-FiLM architecture

The Proposed Architecture



The Modulator receives a time series $\mathbf{x}^{(d)} = \{\mathbf{x}_\tau\}_{\tau=1}^T$ together with static covariates $\mathbf{x}^{(s)}$

The static covariates initialise the hidden state of the GRU encoder through a MLP:

$$\mathbf{h}_0 = \mathrm{MLP}\left(\mathbf{x}^{(s)}\right)$$

Then, the GRU processes the dynamic inputs sequentially:

$$\mathbf{h}_\tau = \mathrm{GRU}\left(\mathbf{x}_\tau^{(d)}, \mathbf{h}_{\tau-1}\right), \qquad \tau = 1, \ldots, T$$

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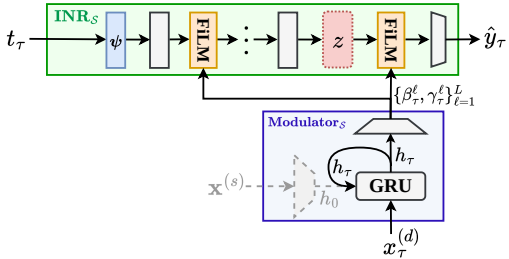

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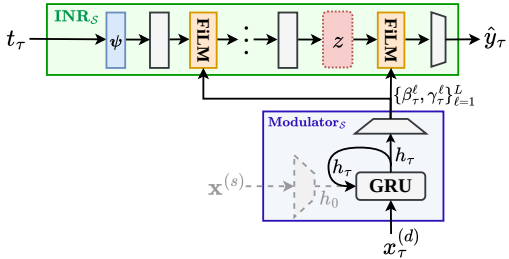

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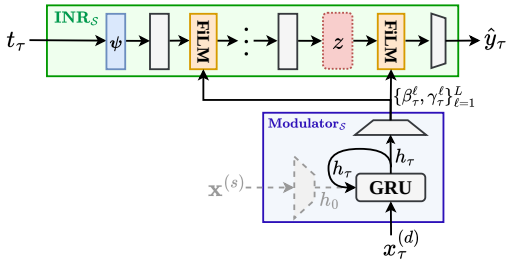

For each layer $\ell = 1, \ldots, L$ of the INR and for each step τ, the modulation parameters are obtained from the current GRU hidden state $\mathbf{h}_\tau$ through linear projections:

$$\boldsymbol{\gamma}_\tau^\ell = \mathbf{W}^{\ell,\gamma}\mathbf{h}_\tau + \mathbf{b}^{\ell,\gamma}, \qquad \boldsymbol{\gamma}_\tau^\ell, \boldsymbol{\beta}_\tau^\ell \in \mathbb{R}^d,$$
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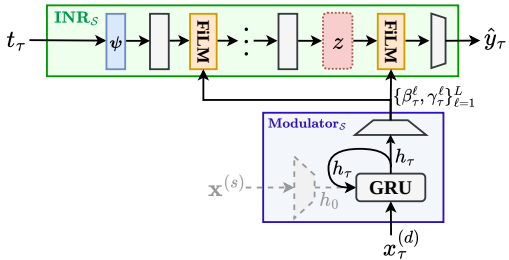

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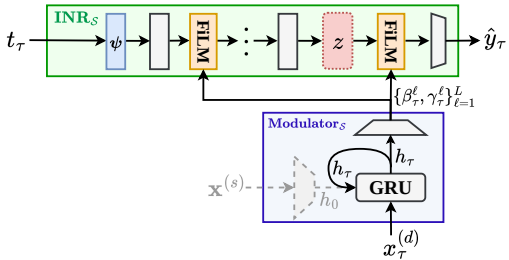

The INR is evaluated independently at each time step t_τ using modulation parameters generated from $\mathbf{h}_\tau$

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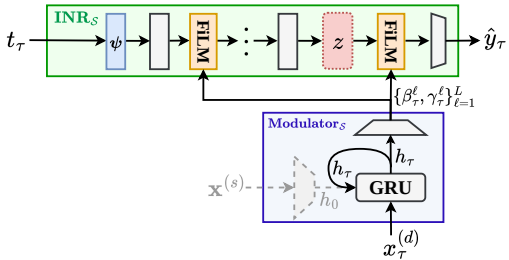
$$\psi(t) = \left[\sin(2^0\pi t), \cos(2^0\pi t), \ldots, \sin(2^{K-1}\pi t), \cos(2^{K-1}\pi t)\right]$$

Mildenhall et al. 2020; Zhong et al. 2020

The Proposed Architecture



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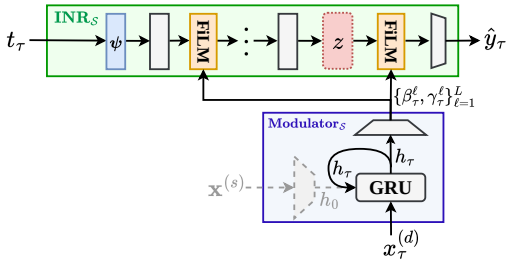

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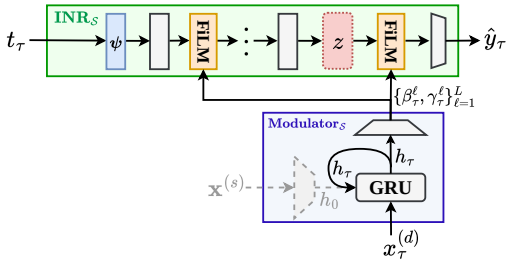

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Then, each of the remaining layers computes:

$$\mathbf{z}_\tau^\ell = \boldsymbol{\gamma}_\tau^\ell \odot \phi\big(\mathbf{W}^\ell \mathbf{z}_\tau^{\ell-1} + \mathbf{b}^\ell\big) + \boldsymbol{\beta}_\tau^\ell, \qquad \ell = 1, \ldots, L,$$

where ϕ denotes the activation function and $\odot$ the element-wise multiplication.

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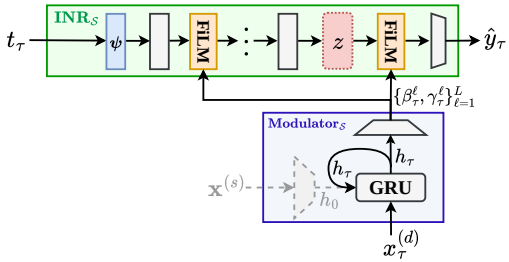

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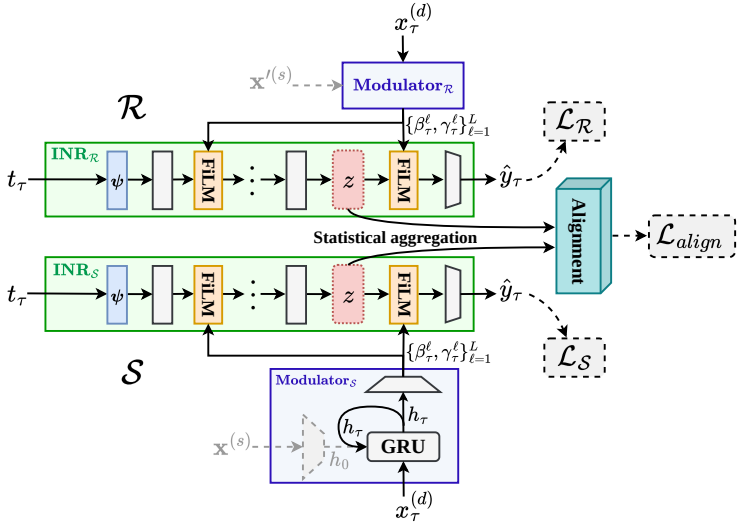


Alignement Techniques

MMD

$$\mathcal{L}_{\text{MMD}} = \mathbb{E}_{x,x'}[k(x,x')] + \mathbb{E}_{y,y'}[k(y,y')] - 2\,\mathbb{E}_{x,y}[k(x,y)]$$

CORAL

$$\mathcal{L}_{\text{CORAL}} = \frac{1}{4d^2}\|C_s - C_r\|_F^2$$

Adv(μ, σ)

$$\mathcal{L}_{\text{adv}} = -\sum_i [y_i \log \sigma(f_i) + (1-y_i)\log(1-\sigma(f_i))]$$

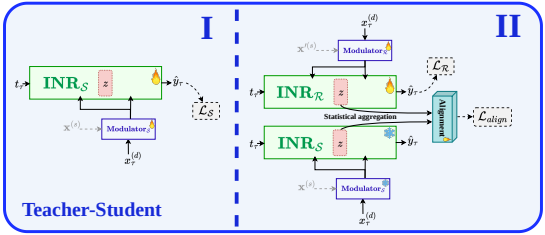
$$f_i = \text{MLP}([\mu_i, \sigma_i]), \quad \mu_i = \frac{1}{B}\sum_b h_b, \quad \sigma_i = \text{std}_b(h_b)$$

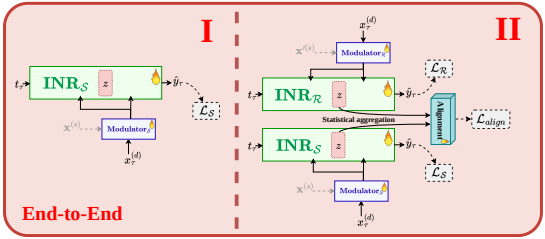
Adv(cov)

$$\mathcal{L}_{\text{adv}} = -\sum_i [y_i \log \sigma(f_i) + (1-y_i)\log(1-\sigma(f_i))]$$

$$f_i = \mathbf{w}^\top \frac{1}{H}\sum_{j=1}^{H} \text{MLP}(\mathbf{C}_i[j,:]), \quad \mathbf{C}_i = \frac{1}{B-1}\tilde{H}_i^\top \tilde{H}_i$$

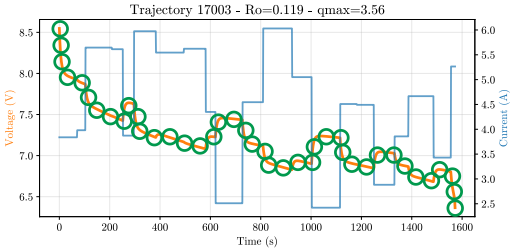
Training Setups



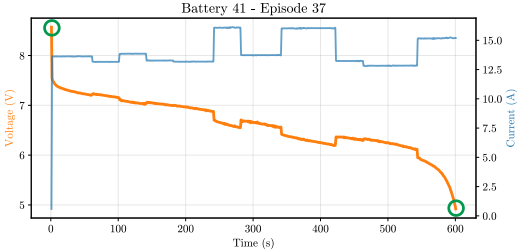


Use Case

Batteries Discharge Curve Prediction



A sample from $D_{\mathcal{S}}$



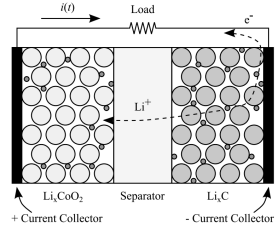
A sample from $D_{\mathcal{R}}$

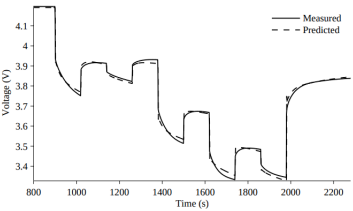
Available y_t for supervision

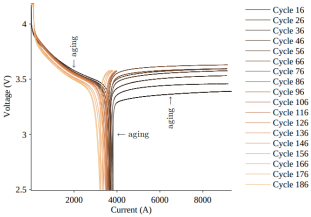
- 20000 samples: 1S, 2S and 3S
- R_0 and $q_{\max}$ (LHS)
- $\mathbf{x}^{(s)} = \{R_0, q_{\max}\}$
- 70/15/15, length $[100 - 3834]$

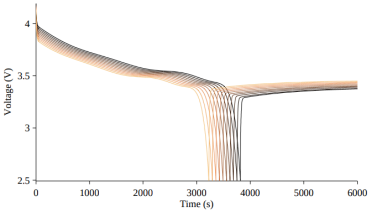
- 4382 samples from 15 batteries (2S)
- $\mathbf{x}^{(s)} = \{\text{Cycle\_number}\}$
- 70/15/15, length $[152 - 3693]$

Electrochemical Simulator



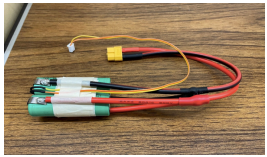


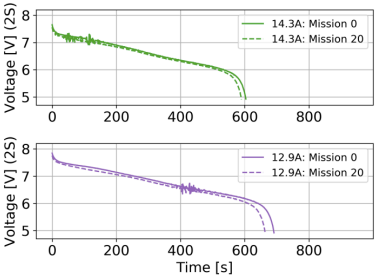




Daigle and Kulkarni 2013

Samsung INR18650-25R





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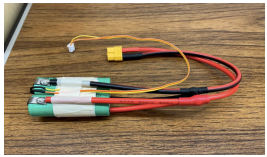

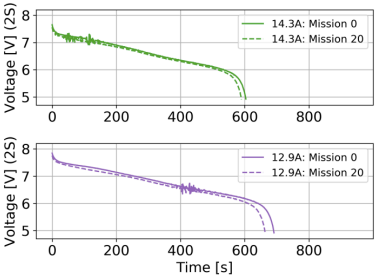

- The batteries are the same model as the ones used for the physical model's default parameters !
- We know the entire voltage sequence
- **Non-uniform time step** and **good representation of sensor artifacts**.

Fricke et al. 2023

Results

Quantitative Results

Alignment method	Simulated Domain $\mathcal{S}$				Real-world Domain $\mathcal{R}$					
	T-S		E2E		T-S			E2E		
	MSE	$\mathbf{V}_{mon}$	MSE	$\mathbf{V}_{mon}$	$\text{MSE}_{\{0,T\}}$	$\mathbf{V}_{mon}$	MSE	$\text{MSE}_{\{0,T\}}$	$\mathbf{V}_{mon}$	MSE
MMD	0.075	0.397	0.084	0.369	9.41e-4	0.380	**0.337**	9.29e-4	0.363	0.301
CORAL	0.074	0.377	0.081	0.397	**7.18e-4**	0.062	0.494	**7.84e-4**	**0.199**	**0.147**
Adv(μ, σ)	0.071	0.333	0.091	0.425	5.65e-4	0.451	0.391	1.98e-3	0.475	0.870
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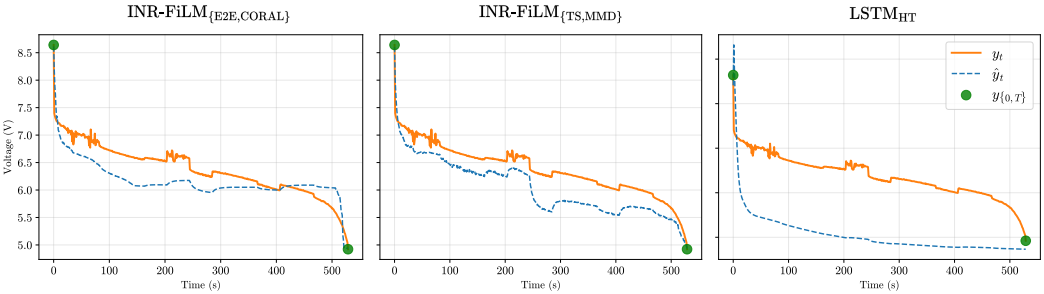
Model	$\text{MSE}_{\{0,T\}}$	MSE
LSTM_{FT}	0.371	1.851
LSTM_{HT}	0.434	1.487
INR_{FT}	0.366	2.968
INR_{mod}	0.363	2.600
$\text{INR} - \text{FiLM}_{\{\text{E2E,CORAL}\}}$ **(Best Ours)**	**7.84e-4**	**0.147**

Qualitative Results



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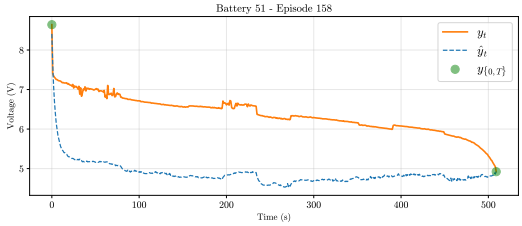

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