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# Towards Accurate Test-Time Adaptation for Neural Surrogates

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## Abstract

1 Neural surrogates that map input configurations (e.g., initial conditions and meshes)  
2 to simulation outputs are increasingly used in practical applications such as en-  
3 gineering design optimization. However, pre-trained models often experience  
4 significant performance drop on unseen problem configurations, such as different  
5 geometries, structural dimensions, and physical parameters. Test-Time Adapt-  
6 ation (TTA) mitigates distribution shifts by leveraging target configurations, online  
7 and at test-time. It avoids the need for costly re-training and doesn't require access  
8 to the original dataset, which is typically unavailable in practice. In this work we  
9 propose Representation Alignment for Simulations (SimRA), a novel method to  
10 improve performance at deployment, specific for multi-dimensional regression  
11 on simulation data. SimRA extends prior work on univariate regression [Adachi  
12 et al., ICLR 2025] with a novel feature weighting mechanism, ensuring stability  
13 in high-dimensional simulation settings. To our knowledge, this is the first study  
14 of TTA for neural surrogates. Empirical evaluations on diverse engineering tasks  
15 demonstrate strong performance and highlight the potential of TTA in the field.

## 16 1 Introduction

17 Neural surrogates have become powerful tools for solving Partial Differential Equation (PDE)  
18 simulations in engineering and science. They perform well when test conditions match the training  
19 data, but performance often drops on novel configurations (geometry, material types, structural  
20 dimensions, and physical parameters), i.e., when the data distribution shifts. This problem often  
21 arises in industrial design optimization, where parameters can vary significantly across iterations and  
22 go beyond the ranges known a priori. Furthermore, in such cases, access to the original source data is  
23 often limited by portability or proprietary restrictions, which makes zero-shot or source-free test-time  
24 adaptation crucial for practical deployment.

25 Several approaches have been proposed to address distribution shifts, including domain gener-  
26 alization [7], meta-learning [16], and active learning [36]. Unfortunately, many of these meth-  
27 ods are impractical for engineering tasks where rapid adaptation is essential. In contrast, Test-  
28 Time Adaptation (TTA) adapts models at inference without source data and with minimal addi-  
29 tional training effort [25, 40, 46]. TTA has proven effective in many domains, including medi-  
30 cal imaging, object detection, and segmentation. While many works are known for classifica-  
31 tion [46, 56, 31, 53, 55, 17, 20, 10, 2, 18], comparably little research can be found for regression [27]. One  
32 outstanding method is Significant-Subspace Alignment (SSA) [3], capable of handling both classifica-  
33 tion and regression tasks. It is however restricted to one-dimensional regression outputs and depends  
34 on manual selection of feature parameters, potentially causing instability for high-dimensional data.

35 Our contributions are summarized as follows:

36 • SimRA is the first TTA method for simulations, to our knowledge. SimRA not only  
37 consistently outperforms SSA, but also eliminates the need for feature pre-selection.

38 • We evaluate TTA on distribution shifts in industrial settings, trying to cover diverse configu-  
39 rations from realistic engineering design scenarios, on SIMSHIFT datasets [35].

40 • Since TTA for physical neural surrogates remains largely unexplored, we identify promising  
41 opportunities for innovation at the intersection of physics and adaptive machine learning.

## 42 2 Related Work

43 **Neural surrogates** have emerged as a widely used approach to accelerate traditional numerical  
44 simulation methods, by providing fast approximations of the solutions. In general, surrogate models  
45 are trained on the solutions from numerical solvers, paired with the corresponding initial conditions  
46 and configurations under which they were generated, e.g., [35, 8, 44, 43]. A particularly prominent  
47 line of work within neural surrogate modeling for PDEs is operator learning [21, 24, 28, 4, 49]. Such  
48 models aim to directly approximate the solution operator that maps initial functions (conditions and  
49 input terms) to output functions.

50 **Test-Time Adaptation (TTA)** refers to the emerging machine learning technique of adapting a pre-  
51 trained model to unlabeled target data, directly at inference time and prior to generating predictions.  
52 For this reason, TTA has recently attracted increasing attention as it offers a (nearly) free performance  
53 gain [27]. While the majority of existing TTA methods have been developed for low-dimensional  
54 classification tasks [26, 51], employing methodologies such as entropy minimization [46, 56, 31, 53,  
55] and feature alignment [17, 20, 10, 2, 18], recent works have begun to extend these ideas to image  
56 segmentation [45, 15, 19]. Research in regression problems is very sparse, and standard TTA methods  
57 cannot be trivially applied. One potential reason is the use of Mean Squared Error in regression  
58 problems, which often leads to a focus on a narrow set of predictive features, reducing diversity [54].  
59 Significant-Subspace Alignment (SSA) [3] addresses these limitations by selecting and aligning the  
60 important feature dimensions, and shows positive performance in the one-dimensional cases. In this  
61 work, we extend and refine SSA for neural surrogates and resolve instability issues arising in the  
62 high-dimensional regression setting. Finally, TTA should not be confused with Test-Time Training  
63 (TTT), often used in time series literature [39, 47, 42, 41]. While both solve the same problem, TTT  
64 typically refers to methods that employ time-series specific techniques, for example updating hidden  
65 states during sequential inference.

66 **Domain generalization, meta-learning, and active learning** represent alternative strategies that  
67 can be used to improve model robustness and generalization under distribution shifts. Domain  
68 generalization [29, 23] and Unsupervised Domain Adaptation (UDA) [38, 14, 52, 13] While effective  
69 in some scenarios, their reliance on specific training, model selection and diverse training distributions  
70 limits their applicability. Meta-learning methods [12] and active learning [22, 30] are similarly  
71 motivated, but generally assume access to ground-truth information in the shifted domain. In our  
72 setting, all these approaches face a significant practical limitation: none of them can quickly adapt a  
73 pre-trained model leveraging unlabeled data at test-time, as they all rely on a priori knowledge and  
74 training. This motivates our exploration of TTA as a more suitable solution.

## 75 3 Problem

76 Following [50, 27], we assume access to a regressor  $f_\theta : \mathcal{X} \rightarrow \mathbb{R}^d$  pre-trained on a *source* sample  
77  $(\mathbf{x}_i, \mathbf{y}_i)_{i=1}^{N^{\text{src}}} \in \mathcal{X} \times \mathbb{R}^d$  drawn from a source distribution  $P^{\text{src}}$ , e.g.,  $f_\theta = g \circ \phi$  in Fig. 1. We also  
78 assume access to some real matrix-valued source statistics  $\Sigma^{\text{src}}, \mu^{\text{src}}, \sigma^{\text{src}}$ .

79 The goal is, for any new *unlabeled* sample  $(\mathbf{x}_i^{\text{tgt}})_{i=1}^{N^{\text{tgt}}}$  drawn from the input marginal of a *target*  
80 distribution  $P^{\text{tgt}} \neq P^{\text{src}}$ , to find  $\theta^{\text{tgt}}$  (using the source statistics but not the source sample) which  
81 minimizes the risk

$$\mathcal{R}(f_\theta) = \frac{1}{N^{\text{tgt}}} \sum_{i=1}^{N^{\text{tgt}}} \|f_\theta(\mathbf{x}_i^{\text{tgt}}) - \mathbf{y}_i^{\text{tgt}}\|_2^2.$$

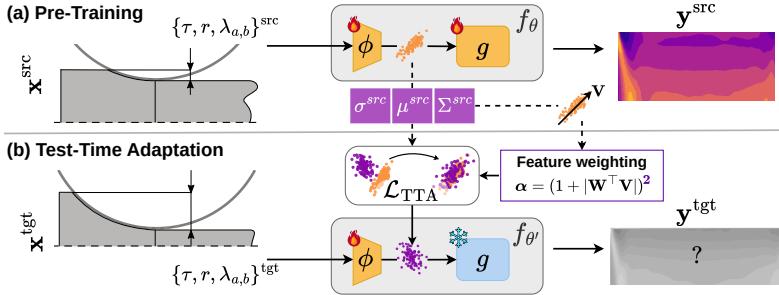


Figure 1: Overview of training and test-time adaptation. (a) Pre-training on the source domain using input parameters: thickness ( $\tau$ ), post-rolling reduction ( $r$ ), and temperature coefficients ( $\lambda_a, \lambda_b$ ). The *representation learner*  $\phi$  and the *predictor*  $g$  are optimized jointly. (b) Test-time adaptation on the target domain, where only the input parameters are available. Here  $\phi$  is adapted and  $g$  is frozen.

82 Note that we have no access to any target labels  $(\mathbf{y}_i^{\text{tgt}})_{i=1}^{N^{\text{tgt}}}$ . That is, the target risk  $\mathcal{R}(f_\theta)$  cannot be  
83 evaluated directly and importance weighting [37] cannot be used without further modification.

84 We study the problem above using the SIMSHIFT benchmark dataset [35], designed to evaluate  
85 how surrogate models adapt to distribution shifts on real-world industrial simulation tasks. In  
86 the benchmark, the inputs  $\mathbf{x}$  represent parameters like geometry, material properties, or operating  
87 conditions, while the labels  $\mathbf{y}$  correspond to high-dimensional fields, such as stresses, deformation  
88 and temperature. The target distribution originates from unseen parameter configurations and the  
89 goal is to predict the corresponding fields.

## 90 4 Method

91 We build on SSA [3], extending it to handle multi-output regression for simulation-based tasks. In  
92 the original formulation, the regression network is divided into two connected parts: a *representation*  
93 *learner*  $\phi$  that produces intermediate features, and a *predictor*  $g$  that maps these features to outputs.  
94 Adaptations occur in the representation stage, while the predictor remains unchanged. Fig. 1 sketches  
95 this process using hot rolling as an example, and distinguishes between (a) pretraining and (b) TTA  
96 with SimRA.

97 The idea is to adjust the features  $\mathbf{z} := \phi(\mathbf{x})$ ,  $\mathbf{z} \in \mathbb{R}^C$  such that the target features are similarly  
98 distributed as the source features. During TTA, target batch statistics are computed on-the-fly, while  
99 source statistics  $\Sigma^{\text{src}}$ ,  $\mu^{\text{src}}$ ,  $\sigma^{\text{src}}$  (pre-computed and stored after training) are used to align the source  
100 and target feature distributions by minimizing the Kullback-Leibler divergence (see Appendix A).

101 A central element of SSA is its *pre-computed significant subspace*, which retains only the dominant  
102 eigenvalues by using a fixed, manually pre-selected subset of  $K$  principal components. Instead, we  
103 use all feature directions and apply *dimension weighting* via exponentiation of the weighting function:

$$\boldsymbol{\alpha} = (1 + |\mathbf{W}^T \mathbf{V}^{\text{src}}|)^2, \quad (1)$$

104 where  $\mathbf{W} \in \mathbb{R}^{K \times C}$  are weights from the first layer of the predictor  $g$  (for a  $C$ -dimensional  $\mathbf{z}$ ) and  
105  $\mathbf{V}^{\text{src}} \in \mathbb{R}^{K \times K}$  is the principal component basis of the source features. Representation alignment is  
106 applied to the target features  $\mathbf{z}^{\text{tgt}} := \phi(\mathbf{x}^{\text{tgt}})$ . Each channel  $\mathbf{z}_c^{\text{tgt}}$  is projected onto the source basis  
107  $\mathbf{V}^{\text{src}}$ , reweighted by the corresponding factor  $\boldsymbol{\alpha}_c$  with  $c \in [0, C - 1]$  as

$$\tilde{\mathbf{z}}_c^{\text{tgt}} = (\mathbf{z}_c^{\text{tgt}} - \mu^{\text{src}}) \mathbf{V}^{\text{src}} \boldsymbol{\alpha}_c, \quad (2)$$

108 where  $\boldsymbol{\alpha}_c$  is the  $c$ -th row of  $\boldsymbol{\alpha}$  (channel-wise). By using Eqs. (1) and (2) to do feature selection,  
109 SimRA can preserve a richer set of features, improving adaptation under distribution shift for

Table 1: Comparison of current baselines with TTA methods for all simulation datasets. Results are averaged across 20 TTA runs, over 2 models (40 seeds in total) with standard deviation reported.

(a) Rolling				(b) Motor			
Model	RMSE (↓)	MAE (↓)	$R^2$ (↑)	Model	RMSE (↓)	MAE (↓)	$R^2$ (↑)
Source	$0.723 \pm 0.046$	$0.419 \pm 0.014$	$0.860 \pm 0.018$	Source	$0.127 \pm 0.002$	$0.061 \pm 0.002$	$0.987 \pm 0.001$
UDA	$0.644 \pm 0.041$	$0.399 \pm 0.012$	$0.869 \pm 0.017$	UDA	$0.119 \pm 0.001$	$0.061 \pm 0.000$	$0.987 \pm 0.001$
SSA	$0.735 \pm 0.097$	$0.441 \pm 0.055$	$0.854 \pm 0.039$	SSA	$0.125 \pm 0.002$	$0.062 \pm 0.002$	$0.986 \pm 0.001$
SimRA	$0.699 \pm 0.064$	$0.418 \pm 0.041$	$0.868 \pm 0.031$	SimRA	$0.124 \pm 0.002$	$0.061 \pm 0.001$	$0.987 \pm 0.001$

(c) Forming				(d) Heatsink			
Model	RMSE (↓)	MAE (↓)	$R^2$ (↑)	Model	RMSE (↓)	MAE (↓)	$R^2$ (↑)
Source	$0.166 \pm 0.020$	$0.055 \pm 0.006$	$0.982 \pm 0.004$	Source	$0.634 \pm 0.012$	$0.424 \pm 0.004$	$0.484 \pm 0.027$
UDA	$0.154 \pm 0.009$	$0.052 \pm 0.003$	$0.984 \pm 0.002$	UDA	$0.577 \pm 0.005$	$0.374 \pm 0.001$	$0.553 \pm 0.002$
SSA	$0.170 \pm 0.026$	$0.057 \pm 0.010$	$0.981 \pm 0.006$	SSA	$0.632 \pm 0.014$	$0.424 \pm 0.003$	$0.484 \pm 0.026$
SimRA	$0.164 \pm 0.018$	$0.054 \pm 0.006$	$0.983 \pm 0.004$	SimRA	$0.631 \pm 0.014$	$0.423 \pm 0.003$	$0.485 \pm 0.026$

110 simulation datasets. Furthermore, since our targets are vector-valued, we compute the Kullback-  
111 Leibler divergence independently for each channel, rather than combining them into a single space.

## 112 5 Experiments

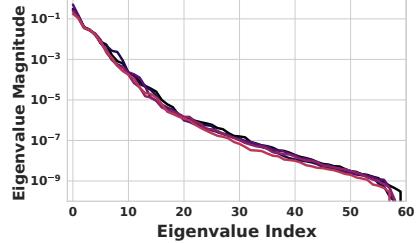
113 **Performance.** To investigate the performance of the proposed method, we use the SIMSHIFT datasets  
114 [35], which span four distinct industrial simulation settings: *hot rolling*, *sheet metal forming*, *electric*  
115 *motor*, and *heatsink design*. All datasets have explicit source and target domain splits, dependent on  
116 the physical and meshing parameters used to generate the samples. Shifts happen in parametric space,  
117 as opposed to unstructured variations occurring in images. For insights into the dataset components  
118 and their creation, please refer to the Appendix of SIMSHIFT [35].

119 Table 1 summarizes the results across all datasets, comparing our method against SSA, "unregu-  
120 larized" pre-trained predictions ("Source"), and Unsupervised Domain Adaptation (UDA) applied  
121 to the pre-trained model. For implementation details refer to Appendix B. SimRA consistently  
122 outperforms SSA, establishing a new baseline for test-time adaptation in neural surrogate regression.  
123 While improvements over the source model may be marginal in some cases, SSA can destabilize  
124 the pre-trained model, whereas our approach does not degrade performance. Moreover, when using  
125 UDA as a lower bound, our method reduces the gap without fully closing it, leaving room for future  
126 improvement.

127 **Interpretation and ablations.** Different datasets can experience varying degrees of improvement  
128 from TTA, highlighting the unique complexities of each problem. By analyzing the eigenvalue  
129 distribution (Fig. 2b for hot rolling), we observe that improvements correlate with the explanatory  
130 power of the leading eigenvalues: datasets where a few components capture most of the variance  
131 exhibit stronger adaptation gains. In contrast, in the motor dataset, variance is spread across many  
132 eigenvalues, indicating a higher-dimensional problem structure and limiting the effectiveness of  
133 current TTA methods. See Appendix C for the full eigenvalue analysis.

134 To illustrate this point, we ablate the impact of the number of dimensions  $K$  of the feature subspace  
135 for the standard SSA algorithm in Fig. 2. Originally,  $K$  has to be chosen manually from the eigenvalue  
136 spectrum of the covariance matrix, requiring expert interaction. While the variance in the hot rolling  
137 datasets decays sharply after the first ten directions (Fig. 2b), several low-variance components  
138 remain correlated with regression targets. SSA results in Fig. 2a suggest that a handpicked  $K$  might  
139 not be optimal, and strict truncation can discard relevant information. For multivariate regression  
140 problems, feature selection is thus critical. Importantly, this choice is absent in SimRA, simplifying  
141 the tuning and yielding superior results. Fig. 2a shows that across different  $K$ -values, our method  
142 always outperforms SSA, irrespective to the chosen subspace size.

Method	$K$	RMSE $\downarrow$	MAE $\downarrow$
SSA	10	0.859 $\pm$ 0.094	0.548 $\pm$ 0.073
	20	0.735 $\pm$ 0.097	0.441 $\pm$ 0.055
	30	0.736 $\pm$ 0.067	0.441 $\pm$ 0.036
	50	0.774 $\pm$ 0.057	0.467 $\pm$ 0.032
	All	0.827 $\pm$ 0.043	0.508 $\pm$ 0.085
SimRA (ours)	All	<b>0.699<math>\pm</math>0.064</b>	<b>0.418<math>\pm</math>0.041</b>



(a) Comparison of SimRA with SSA for different choices of  $k$ .

(b) Eigenvalue analysis.

Figure 2: Ablations with SSA [3] for the hot rolling dataset. (a) table with quantitative comparison, (b) eigenvalues analysis for different trained models, highlighting the fast decay.  $\sim$ 60 % of the energy is on the first eigenvalues, favoring compact representations.

## 143 6 Conclusion and Future Work

144 In this work, we make the initial step towards highly-accurate test-time adaptation methods for neural  
 145 surrogates, and in general for high-dimensional multivariate regression. Our findings show that the  
 146 proposed adjustments enable TTA to yield zero-shot improvements at negligible computational cost.  
 147 Furthermore, the current state-of-the-art method, SSA [3], can be substantially simplified, removing  
 148 the need for feature preselection, while also achieving improved performance and stability. The  
 149 promotion can be interpreted via eigen-decomposition analysis of the feature space, offering insights  
 150 into why our approach outperforms existing methods on the evaluated datasets.

151 In addition to the zero-cost gains, this line of research is particularly timely due to evolving compliance  
 152 requirements. Article 15 of the EU Artificial Intelligence Act states that high-risk AI systems need to  
 153 ensure appropriate levels of accuracy and robustness [1]. Should neural surrogates be deployed in  
 154 safety critical domains, such as accelerating structural design in the automotive industry, accurate  
 155 and reliable predictions becomes indispensable.

156 However, performance improvements only occur on some datasets, and the lower bounds established  
 157 by UDA indicate that additional gains remain attainable. This points to the potential for a new class of  
 158 TTA algorithms, specifically developed for physics simulation data. We foresee two paths to achieve  
 159 "physics-driven" TTA that are to be explored: (i) use physics-informed constraints and priors [34, 9],  
 160 ad-hoc and calibrated on the test case, to augment the expressiveness of the limited available test data,  
 161 and (ii) incorporate uncertainty quantification to localize failure regions in the fields where adaptation  
 162 is necessary. Orthogonally, exploring the impact of TTA in data-driven design optimization [11, 6, 33]  
 163 represents another promising avenue for research. A concrete example would be the *EngiBench*  
 164 dataset [11], which provides a standardized machine learning benchmark for engineering design.

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344 **A Supplementary Approach Information**

345 **Significant-Subspace Alignment** is a TTA method for one-dimensional regression. It consists of  
 346 two steps: *feature alignment* and *significant-subspace alignment*. In the first step, source statistics  
 347 such as mean  $\mu^{\text{src}}$  and covariance  $\Sigma^{\text{src}}$  are computed after source training. In the second step, a  
 348 significant subspace is detected by selecting the top eigenvalues  $\lambda_k$  of the source covariance  $\Sigma^{\text{src}}$ .  
 349 Each subspace direction  $v_k^{\text{src}}$  is then weighted by its influence on the regression output:

$$\alpha_k = 1 + |\mathbf{w}^\top \mathbf{v}_k^{\text{src}}|,$$

350 where  $\alpha_k \geq 1$  ensures that dimensions that strongly affect the regression output are emphasized.  
 351 At test time, the precomputed source statistics are used to project the target features into the significant  
 352 subspace. From the projected target features, their mean and variance  $(\tilde{\mu}_k^{\text{tgt}}, \tilde{\sigma}_k^{\text{tgt}2})$  are calculated  
 353 and aligned with the corresponding source statistics  $(0, \lambda_k^{\text{src}})$ . The adaptation objective is a weighted  
 354 symmetric Kullback-Leibler divergence between assumed Normal distributions:

$$\mathcal{L}_{\text{TTA}} = \frac{1}{2} \sum_{k=1}^K \alpha_k \left( \frac{(\tilde{\mu}_k^{\text{tgt}})^2 + \lambda_k^{\text{src}}}{\tilde{\sigma}_k^{\text{tgt}2}} + \frac{(\tilde{\mu}_k^{\text{tgt}})^2 + \tilde{\sigma}_k^{\text{tgt}2}}{\lambda_k^{\text{src}}} - 2 \right). \quad (3)$$

355 **B Experimental Setup**

356 In the following paragraphs, we detail the experimental setup, including the selected models and our  
 357 training and testing strategy, based on established methods [3].

358 **B.1 Model Architecture**

359 We employ a single model architecture to evaluate our TTA method. The model is taken from the  
 360 SIMSHIFT benchmark [35], implemented in PyTorch, and designed for conditional regression. Node  
 361 coordinates are provided as inputs and embedded using sinusoidal positional encodings. Conditioning  
 362 is applied through a dedicated network that processes the simulation input parameters.

363 **Conditioning Network.** The conditioner maps simulation parameters into a latent representation  
 364 of dimension 8. It consists of a sinusoidal encoding, followed by a small MLP, which includes two  
 365 LayerNorms to stabilize training.

366 **Transolver.** The Transolver architecture [48] starts by encoding node coordinates using sinusoidal  
 367 position embeddings, followed by an MLP that produces initial feature vectors. A learned mapping  
 368 then assigns each node to a slice, enabling attention operations both within slices and between them.  
 369 The processed features are passed through an MLP readout to generate the final field outputs. Two  
 370 conditioning mechanisms are available: concatenating the conditioning vector with input features or  
 371 applying it via DiT-based modulation across the network. Conditioning is done with the dit-based  
 372 modulation [32]. Where a latent dimension of 128, a slice base of 32, and four attention layers  
 373 are used. We additionally employ a larger model with 56, 128, and 8 layers for the more complex  
 374 datasets.

375 **B.2 Test-Time Adaptation Setup**

376 In our experiments, we train baseline models for each dataset on 2 seeds, using the training pipeline  
 377 from SIMSHIFT. We employ the small model variants for hot rolling, electric motor design, and sheet  
 378 metal forming, and the large model variant for the more complex heatsink. For the TTA experiments,  
 379 we utilize source test data to compute statistical information, then adapt and evaluate the models on  
 380 target test data. The implementation of TTA follows the algorithmic framework provided in the SSA  
 381 repository, with modifications described in Section 4. The adaptation process is limited to a single  
 382 epoch, as in [3].

383 In our specific setup, task-dependent parameters, such as thickness or temperature, are encoded  
 384 through a conditioner network. The conditioner is divided into two components: a main body and  
 385 a final linear layer. We extract features from the main body’s output and define the split between  
 386 representation learner and predictor at this point—the conditioner serves as the representation learner,

387 while Transolver acts as the predictor. This choice reflects the observation that most task-related  
 388 parameter shifts occur within the conditioner [35]. For training SimRA we modify the weighted  
 389 symmetric Kullback-Leibler divergence from Eq. (3) to account for Eq. (2) by removing  $\alpha_k$

$$\mathcal{L}_{\text{TTA}} = \frac{1}{2} \sum_{k=1}^K \left( \frac{(\tilde{\mu}_k^{\text{tgt}})^2 + \lambda_k^{\text{src}}}{\tilde{\sigma}_k^{\text{tgt}2}} + \frac{(\tilde{\mu}_k^{\text{tgt}})^2 + \tilde{\sigma}_k^{\text{tgt}2}}{\lambda_k^{\text{src}}} - 2 \right). \quad (4)$$

390 During testing, we adapt only the layer normalization [5] parameters of the conditioner, keeping all  
 391 other model parameters fixed. To ensure robustness, we repeat each experiment with 20 different  
 392 random seeds per model. This is particularly important since layer normalization is updated online,  
 393 after every batch. All experiments are conducted with a fixed batch size of 32.

394 For comparison, we also report the best performing UDA algorithm as a lower bound. These models  
 395 are trained according to the procedure outlined in SIMSHIFT [35]. We run the DeepCoral algorithm  
 396 [38] with the provided  $\lambda$  ranges. After applying selection and emsembling strategies on top of the  
 397 UDA algorithm, we showcase the best-performing model for each dataset. It is important to note  
 398 that the UDA training process requires significantly more compute budget than the TTA approach:  
 399 instead of requiring a single pre-trained model, UDA model selection relies on multiple models for  
 400 robustness, each trained independently with different  $\lambda$  values.

## 401 C Additional results

402 To investigate the difference in effectiveness of TTA algorithms to different datasets, we analyze  
 403 the features extracted by the representation learner. Specifically, the eigenvalue spectra of the  
 404 corresponding covariance matrices are compared for each dataset. In Fig. 3, the eigenvalues for three  
 405 out of four datasets (hot rolling, sheet metal forming, and heatsink design) show a similar decay:  
 406 the first five eigenvalues already capture up to  $\sim 60\%$  of the total variance. This is also confirmed  
 407 by Table 2. In contrast, the electric motor dataset exhibits a much slower decay, suggesting that  
 408 the variance is distributed across a larger number of components. This implies that electric motor  
 409 requires a higher-dimensional representation to preserve the same level of information, whereas the  
 410 other datasets are more efficiently represented in a low-dimensional manifold.

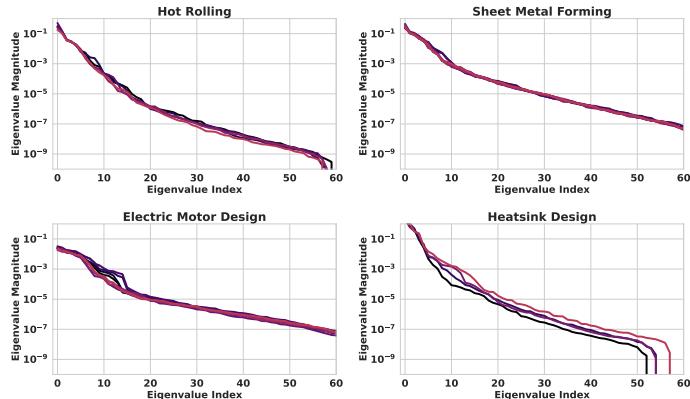


Figure 3: Eigenvalues analysis of *hot rolling*, *sheet metal forming*, *electric motor* and *heatsink design*, expressing the diverging decay throughout the datasets.

Table 2: Percentage of variance explained by the top 10 eigenvalues for each dataset.

Dataset	$\lambda_0$	$\lambda_1$	$\lambda_2$	$\lambda_3$	$\lambda_4$	$\lambda_5$	$\lambda_6$	$\lambda_7$	$\lambda_8$	$\lambda_9$
Rolling	57.9 %	23.6 %	7.1 %	5.4 %	3.4 %	1.4 %	0.7 %	0.3 %	0.2 %	0.1 %
Forming	47.6 %	18.3 %	14.2 %	8.6 %	5.6 %	3.0 %	1.3 %	0.8 %	0.4 %	0.2 %
Motor	25.0 %	19.5 %	15.2 %	13.2 %	10.4 %	7.6 %	4.3 %	2.7 %	1.3 %	0.7 %
Heatsink	63.9 %	22.3 %	8.5 %	4.2 %	0.5 %	0.2 %	0.1 %	0.1 %	0.0 %	0.0 %