WHICH MODEL TO TRANSFER? FINDING THE NEEDLE IN THE GROWING HAYSTACK

Cedric Renggli*André Susano PintoLuka RimanicJoan PuigcerverETH ZurichGoogle ResearchETH ZurichGoogle Research

Carlos RiquelmeCe ZhangMario LucicGoogle ResearchETH ZurichGoogle Research

ABSTRACT

Transfer learning has been recently popularized as a data-efficient alternative to training models from scratch, in particular in vision and NLP where it provides a remarkably solid baseline. The emergence of rich model repositories, such as TensorFlow Hub, enables the practitioners and researchers to unleash the potential of these models across a wide range of downstream tasks. As these repositories keep growing exponentially, efficiently selecting a good model for the task at hand becomes paramount. We provide a formalization of this problem through a familiar notion of *regret* and introduce the predominant strategies, namely *task-agnostic* (e.g. picking the highest scoring ImageNet model) and *task-aware* search strategies (such as *linear* or *kNN* evaluation). We conduct a large-scale empirical study and show that both task-agnostic and task-aware methods can yield high regret. We then propose a simple and computationally efficient hybrid search strategy which outperforms the existing approaches. We highlight the practical benefits of the proposed solution on a set of 19 diverse vision tasks.

1 Introduction

Services such as TensorFlow Hub^1 or PyTorch Hub^1 offer a plethora of pre-trained models that often achieve state-of-the-art performance on specific tasks in the vision and NLP domains. The predominant approach, namely choosing a pre-trained model and *fine-tuning* it to the downstream task, remains a very strong and data efficient baseline. This approach is not only successful when the pre-training task is similar to the target task, but also across tasks with seemingly differing characteristics, such as applying an ImageNet pre-trained model to medical applications like diabetic retinopathy classification (Oquab et al., 2014). Fine-tuning often entails adding several more layers to the pre-trained deep network and tuning all the parameters using a limited amount of downstream data. Due to the fact that all parameters are being updated, this process can be extremely costly and intensive in terms of compute (Zhai et al., 2019). Fine-tuning all models to find the best performing one is rapidly becoming computationally infeasible. A more efficient alternative is to simply train a linear classifier or a k-nearest neighbour (kNN) classifier on top of the learned representation (e.g. pre-logits). However, the performance gap with respect to fine-tuning can be rather large (Kolesnikov et al., 2019; Kornblith et al., 2019).

In this paper we study the application of *computationally efficient methods for determining which model(s) one should fine-tune for a given task at hand*. We divide existing methods into two groups: (a) *task-agnostic* model search strategies – which rank pre-trained models independently of the downstream task (e.g. sort by ImageNet accuracy, if available), and (b) *task-aware* model search strategies – which make use of the provided downstream dataset in order to rank models (e.g. *k*NN classifier accuracy as a proxy for fine-tuning accuracy) (Kornblith et al., 2019; Meiseles & Rokach, 2020; Puigcerver et al., 2020).

Clearly, the performance of these strategies depends on the set of models considered and the computational constraints of the practitioner (e.g. the memory footprint, desired inference time, etc.).

^{*}Work done while interning at Google Research.

Correspondence to Cedric Renggli (cedric.renggli@inf.ethz.ch) and Mario Lucic (lucic@google.com).

¹https://tfhub.dev and https://pytorch.org/hub

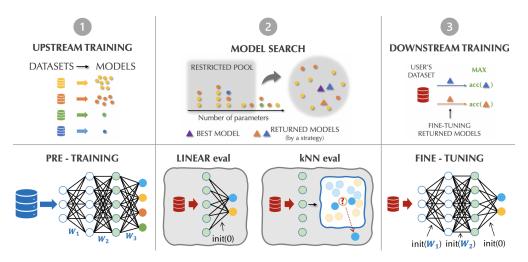


Figure 1: Transfer learning setup: (1) **Upstream models** Pre-training of models from randomly initialized weights on the (large) upstream datasets; (2) **Model search** Downstream task independent, or by running a proxy task, i.e. fixing the weights of all but the last layer and training a *linear classifier* or deploying a *kNN classifier* on the downstream dataset; (3) **Downstream training** Unfreezing all the weights, optimizing the pre-defined and a new linear classification layer on the users task.

To this end, we define several *model pools* and study the performance and generalization of each strategy across different pools. In particular, we make sure that these pools contain both "generalist" models (e.g. models trained on ImageNet), but also "expert" models (e.g. models trained on domain-specific datasets, such as flowers, animals, etc.).

Our contributions. (i) We formally define and motivate the model search problem through a notion of regret. We conduct the first study of this problem in a realistic setting focusing on heterogeneous model pools. (ii) We perform a large-scale experimental study by fine-tuning 19 downstream tasks on 46 models from a heterogeneous set of pre-trained models split into 5 meaningful and representative pools. (iii) We highlight the dependence of the performance of each strategy on the constrained model pool, and show that, perhaps surprisingly, both task-aware and task-agnostic proxies fail (i.e. suffer a large regret) on a significant fraction of downstream tasks. (iv) Finally, we develop a hybrid approach which generalizes across model pools as a practical alternative.

2 BACKGROUND AND RELATED WORK

We will now introduce the main concepts behind the considered transfer learning approach where the pre-trained model is adapted to the target task by learning a mapping from the intermediate representation to the target labels (Pan & Yang, 2009; Tan et al., 2018; Wang, 2018; Weiss et al., 2016), as illustrated in Figure 1.

- (I) Upstream models. Upstream training, or *pre-training*, refers simply to a procedure which trains a model on a given task. Given the variety of data sources, losses, neural architectures, and other design decisions, the set of upstream models provides a diverse set of learned representations which can be used for a downstream task. In general, the user is provided with these models, but can not control any of these dimensions, nor access the upstream training data. Previous work call the models in these pools *specialist* models (Ngiam et al., 2018) or *experts* (Puigcerver et al., 2020). (II) Model search. Given no limits on computation, the problem is trivial exhaustively fine-tune each model and pick the best performing one. In practice, however, one is often faced with stringent requirements on computation, and more efficient strategies are required. The aim of the second stage in Figure 1 is therefore to select a small number of models from the pool, so that they can be fine-tuned in the last step. The central research question of this paper is precisely how we can choose the most promising models for the task at hand.
- (II A) Task-agnostic search strategies. These strategies rank models without looking at the data of the downstream task (Kornblith et al., 2019). As a consequence, given a fixed pool of candidates, the same model is recommended for *every* task. We focus on the following popular task-agnostic approach: (i) Pick the highest test accuracy ImageNet model (if such a model is in the pool), otherwise (ii) pick the one trained on the largest dataset. If there is a tie, pick the biggest model in the pool (in terms of the number of parameters).

(II B) Task-aware search strategies. In contrast to the task-agnostic approach, task-aware ones guide the model selection strategy by using the downstream data. As a result, these strategies require additional computation. In this work we consider the following strategies: Given a model, we first compute and freeze the representations extracted from the last layer for each example in the target dataset. Then, we use a simple classification method to solve the task with the new features provided by the pre-trained model. Finally, we select the models offering highest accuracy in this simplified setup. We focus on two classification methods: a linear classifier, and a k-nearest neighbours classifier. We note that both are usually several orders of magnitude faster than fine-tuning the whole model. In addition, kNN is non-parametric, and it can capture non-linear relationships.

Alternatively, one can *blend* the source and target data by reweighting the upstream data to reflect its similarity to the downstream task (Ngiam et al., 2018), or construct a joint dataset by identifying subsets of the upstream data that are well-aligned with the downstream data (Ge & Yu, 2017). These approaches are less practical as they necessitate training a new model as well as access to upstream datasets which might not be available due to proprietary or privacy concerns. Best-arm identification bandits algorithms suggest the successive elimination of sub-optimal choices (Even-Dar et al., 2006) by potentially fine-tuning full models; note this combines model-selection and downstream training. Recently, Meiseles & Rokach (2020) introduced the Mean Silhouette Coefficient (MSC) to forecast a model's performance after fine-tuning. This approach is omitted in this work due to its provable relation to a linear classifier proxy, and relation to the kNN non-parametric proxy task in terms of ability to capture non-linear relationships. kNN is also utilized by Puigcerver et al. (2020) as a cheap proxy task for searching models in a set of experts with the same architecture.

(III) Downstream training. In this stage, the selected model is adapted to the downstream task (cf. Figure 1). The predominant approach is to fully or partially apply the pre-trained neural network as a feature extractor. The head (e.g. last linear layer) of the pre-trained model is replaced with a new one, and the whole model is trained on the target data. This process is commonly referred to as *fine-tuning* and it often outperforms other methods (Oquab et al., 2014; Donahue et al., 2014; Sharif Razavian et al., 2014; Kornblith et al., 2019).

3 COMPUTATIONAL BUDGET AND REGRET

The main aim of this work is the study of simple methods to filter and search pre-trained models before stepping into the –more expensive– fine-tuning process. Formally, we define a search method $m(\mathcal{M},\mathcal{D})$ with budget B as a function which takes a set of models \mathcal{M} and a downstream dataset \mathcal{D} as input, and outputs a number of distinct models $\mathcal{S}_m \subseteq \mathcal{M}$, with $|\mathcal{S}_m| = B$. Those B models are then all fine-tuned in order to obtain the best possible test accuracy on the downstream task \mathcal{D} .

Budget and regret. Fine-tuning represents the largest computational cost; accordingly, we define the *number* of models that are fine-tuned as the computational complexity of a given method. Given any fixed budget B, we would like to return a set $\mathcal S$ which includes the models resulting in good performance downstream. In particular, we define the notion of *absolute regret* of a search strategy m and a pool of models $\mathcal M$ on dataset $\mathcal D$ as

$$\underbrace{\max_{m_i \in \mathcal{M}} \mathbf{E}[t(m_i, \mathcal{D})]}_{\text{ORACLE}} - \underbrace{\mathbf{E}\left[\max_{s_i \in \mathcal{S}_m} t(s_i, \mathcal{D})\right]}_{s(m)},\tag{1}$$

where $t(m,\mathcal{D})$ is the test accuracy achieved when fine-tuning model m on dataset \mathcal{D} . The first expectation is taken over the randomness in the $t(\cdot)$ operator, that is, the randomness in fine-tuning and due to a finite sampled test set. In addition to the randomness in $t(\cdot)$, the second expectation also accounts for any potential randomization in the algorithm that computes \mathcal{S}_m . We define s(m) as the expected maximal test accuracy achieved by any model in the set \mathcal{S}_m , the set of models returned by a fixed strategy m. In our case, kNN is deterministic as all the downstream data is used, whereas the linear model depends on the randomness of stochastic gradient descent. To enable comparability between datasets of different difficulty as well as a comparison between two selection strategies m_1 , and m_2 , we define their relative delta as

$$\Delta(m_1, m_2) := \frac{s(m_1) - s(m_2)}{1 - \min(s(m_1), s(m_2))},\tag{2}$$

with $s(\cdot) \in [0,1]$ as defined in Equation 1. Substituting $s(m_1)$ by the ORACLE value, and $s(m_2)$ by s(m) leads to the *relative regret* r(m). We discuss the impact of alternative notions in Section 5.4.

4 EXPERIMENTAL DESIGN

Our goal is to assess which model strategies achieve low regret when presented with a diverse set of models. As discussed, there are three key variables: (i) The set of downstream tasks, which serve as a proxy for computing the expected regret of any given strategy, (ii) the *model pool*, namely the set we explore to find low-regret models, and (iii) the transfer-learning algorithms.

4.1 Datasets and models

Datasets. We use VTAB-1K, a few-shot learning benchmark composed of 19 tasks partitioned into 3 groups – •natural, •specialized, and •structured (Zhai et al., 2019). The natural image tasks include images of the natural world captured through standard cameras, representing generic objects, fine-grained classes, or abstract concepts. Specialized tasks contain images captured using specialist equipment, such as medical images or remote sensing. The structured tasks are often derive from artificial environments that target understanding of specific changes between images, such as predicting the distance to an object in a 3D scene (e.g. DeepMind Lab), counting objects (e.g. CLEVR), or detecting orientation (e.g. dSprites for disentangled representations). Each task has 800 training examples, 200 validation examples, and the full test set. This allows us to evaluate model search strategies on a variety of tasks and in a setting where transfer learning offers clear benefits with respect to training from scratch (Zhai et al., 2019).

Models. The motivation behind the model pools is to simulate several use-cases that are ubiquitous in practice. We first collect 46 classification models (detailed overview in Appendix A):

- 15 models trained on the ILSVRC 2012 (ImageNet) classification task (Russakovsky et al., 2015) including Inception V1-V3 models (Szegedy et al., 2016), ResNet V1 and V2 (depth 50, 101, and 152) (He et al., 2016), MobileNet V1 and V2 (Howard et al., 2017), NasNet (Zoph et al., 2018) and PNasNet (Liu et al., 2018) networks.
- 16 ResNet-50-V2 models trained on (subsets of) JFT (Puigcerver et al., 2020). These models are trained on different subsets of a larger dataset and perform significantly better on a small subset of downstream tasks we consider (i.e. they can be considered as *experts*).
- 15 models from the VTAB benchmark², with a diverse coverage of losses (e.g. generative, self-supervised, self-supervised combined with supervised, etc.) and architectures. In all cases the upstream dataset was ImageNet, but the evaluation was performed across the VTAB benchmark which does not include ImageNet.

4.2 Model pools

- (A) Identifying good resource-constrained models (RESNET-50, DIM2048). Here we consider two cases: (i) RESNET-50: All models with the number of parameters smaller or equal to ResNet50-V2. While the number of parameters is clearly not the ideal predictor, this set roughly captures the models with limited memory footprint and inference time typically used in practice. Most notably, this pool excludes the NasNet and PNasNet architectures, and includes the *expert* models. (ii) DIM2048: The transfer strategies discussed in Section 2 might be sensitive to the size of the representation. In addition, restricting the representation size is a common constraint in practical settings. Hence, we consider a model pool where the representation dimension is limited to a maximum of 2048.
- **(B)** Identifying expert models in presence of non-experts (EXPERT). We consider a pool of 16 ResNet-50-V2 models from Puigcerver et al. (2020). These models which we considered as *experts* are trained on different subsets of a larger dataset. As the number of available models and the upstream training regimes increase, the number of such experts is likely to increase. As such, this presents a realistic scenario in which an expert for the target task may be present, but it is hard to identify due to the presence of other models, some of which might perform well *on average*.
- (C) Do better task-agnostic models transfer better (IMNETACCURACIES)? This pool offers the ability to choose an upstream representation-learning technique that is best suited for a specific downstream task. This pool is mainly used to validate the idea that (a) ImageNet models transfer

²https://tfhub.dev/vtab

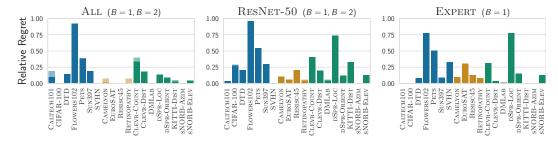


Figure 2: **Task-agnostic strategies.** Relative regret (r(m), cf. Section 3) with B=1 (transparent) and B=2 (solid) on the ALL, RESNET-50 and EXPERT pools, bearing in mind that there is only one task-agnostic model in EXPERT. By definition, task-agnostic strategies exclude experts yielding high regret on the RESNET-50 and EXPERT pools, particularly on natural or structured datasets.

well across different tasks (Huh et al., 2016; He et al., 2019) and that (b) better ImageNet models transfer better (Kornblith et al., 2019).

(D) All models (ALL). Finally, we consider the hardest setting, namely when the model pool contains all 46 models and no conceptual nor computational restrictions are in place. We note that: $EXPERT \subset RESNET-50 \subset DIM2048 \subset ALL$ and $IMNETACCURACIES \subset ALL$.

4.3 EVALUATION PROCEDURES

Fine tuning. To assign a downstream test accuracy to each pair of model and task, we use the median test performance of 5 models obtained as follows: (i) Add a linear layer followed by a softmax layer and train a model on all examples of the training set. (ii) Fine-tune the obtained model twice, considering two learning rates, and 2500 steps of SGD and a batch size of 512 (Zhai et al., 2019). (iii) Return the model with the highest validation accuracy. Note that in this case, the entire model, and not only the linear layer, is retrained. As a result, there are 10 runs for each model and we obtain 8740 trained models $(46 \times 19 \times 5 \times 2)$.

Linear evaluation. We train a logistic regression classifier added to the model representations (fixed) using SGD. We consider two learning rates (0.1 and 0.01) for 2500 steps and select the model with the best validation accuracy. For robustness we run this procedure 5 times and take the median validation accuracy out of those resulting values. As a result, we obtain again 8740 models.

 $k\mathbf{NN}$ evaluation. We compute the validation accuracy by assigning to each of the 200 validation samples the label of the nearest training example (i.e. k=1) using standard Euclidean distance.

5 KEY EXPERIMENTAL RESULTS

In this section we challenge common assumptions and highlight the most important findings of this study, whilst the extended analysis containing all the plots and tables can be found in the supplementary material. We remark that in the main body we only consider three main pools of models – ALL, RESNET-50 and EXPERT, as we see them as the most representative ones. Since DIM2048 behaves very similarly to RESNET-50, whereas IMNETACCURACIES is used only to confirm the findings of Kornblith et al. (2019), the results of ablation studies involving these two pools can be found in Appendix D. Finally, in this section we mainly investigate linear evaluation as the task-aware choice; all the corresponding plots for kNN can be found in Appendix E.

5.1 HIGH REGRET OF TASK-AGNOSTIC STRATEGIES

Figure 2 shows the results for task-agnostic methods with budget B=1 and B=2 on the ALL, RESNET-50, and EXPERT pools. We observe a significant regret, in particularly for RESNET-50 and EXPERT pools (30% of the datasets have a relative regret larger than 25% on those two pools). This highlights the fact that task-agnostic methods are not able to pick expert models, in particular on natural and structured datasets. As more experts become available, this gap is likely to grow, making it clear that task-agnostic strategies are inadequate on its own.

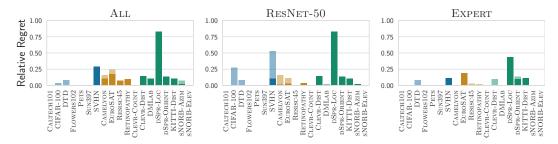


Figure 3: Task-aware strategies (linear). Relative regret for B=1 (transparent) and B=2 (solid) on the ALL, RESNET-50, and EXPERT pools. Compared to task-agnostic strategies, we observe improvement on natural datasets (except SVHN) and on restricted pools (except DSPR-LOC), due to its ability to properly choose experts.

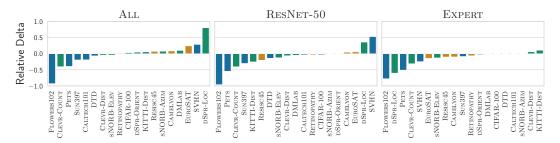


Figure 4: **Task-agnostic** (positive if better) **vs Task-aware** (**linear**) (negative if better) for B=1. On the ALL pool, the methods perform in a similar fashion, with respect to the number of datasets and the amount in which one outperforms the other. When one restricts the pool to RESNET-50 or EXPERT task-aware methods outperform the task-agnostic method on most datasets. The relative delta is defined in Equation 2 in Section 3.

5.2 Are task-aware always a good predictor?

Intuitively, having access to the downstream dataset should be beneficial. We evaluate both the linear and the kNN predictor as detailed in Section 4. Figure 3 provides our overall results for the linear model, whereas analogous results for kNN are presented in Appendix E. The method struggles on some structured datasets (in particular on DSPR-LOC).

Compared to the task-agnostic strategy, as presented in Figure 4 for B=1, we observe significant improvements on restricted model pools. The EXPERT pool benefits the most: linear evaluation outperforms task-agnostic methods on almost every dataset (task-aware is only outperformed on three datasets by more than 1%, and by 10% in the worst case on the KITTI-DIST dataset). On the other hand, task-agnostic and task-aware strategies seem to outperform each other on a similar number of datasets and by a comparable magnitude in the ALL pool. This suggests that no single strategy uniformly dominates all other strategies across pools.

In order to understand this further, we perform an ablation study where we plot the linear and $k{\rm NN}$ regret on the IMNETACCURACIES pool in Appendix D. In Figures 14 and 15 we observe that task-aware search methods perform rather poorly when having access only to different architectures trained on the same upstream data. The IMNETACCURACIES models are included in the ALL pool, and in some datasets some of those models are the best-performing ones.

Performance of the kNN predictor is on par on half of the datasets across the pools, and slightly worse than linear evaluation on the other half. We present these findings in Figure 19 in Appendix E.

5.3 Hybrid approach yields the best of both worlds

A hybrid approach that selects both the top-1 task-agnostic model and the top-(B-1) task-aware models leads to strong overall results. Figure 5 shows how the hybrid approach with linear evaluation as the task-aware method significantly outperforms its linear counterpart with B=2. This is most noticeable in the ALL pool where the task-agnostic model provides a large boost on some datasets.

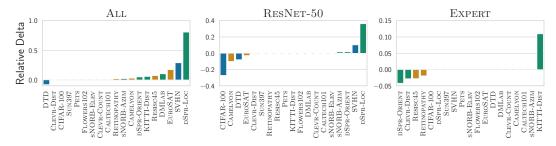


Figure 5: **Hybrid linear** (positive if better) **vs Linear evaluation** (negative if better) for B=2. We observe that hybrid linear significantly outperforms linear with the same budget on the ALL pool. Even though for RESNET-50 and EXPERT pools there are datasets on which linear performs better than hybrid, the amounts in which it does are usually small. We note that most significant gains of hybrid come on certain structured datasets, the hardest task for every strategy.

As we saw in Figure 4, when looking at the ALL pool, the task-agnostic candidate tends to beat the linear one on datasets such as DSPR-LOC, SVHN or EUROSAT. Similarly, the linear candidate model clearly outperforms its task-agnostic counterpart on many natural datasets such as FLOWERS or PETS. A comparison of Figures 4 and 5 reflects how the dominance of linear-only strategy vanishes on most datasets when confronted with the hybrid approach. For the RESNET-50 and EXPERT pools, as expected, the hybrid algorithm preserves the good picks of the linear proxy. That said, we observe an increase of 36% on DSPR-LOC in the RESNET-50, and 11% on KITTI-DIST. Both are structured datasets on which the linear proxy task performs poorly, as shown in Figure 3.

The hybrid strategy requires to fine-tune at least two models. Given that it performs well across all model pools and datasets, this is a reasonable price to pay in practice, and we suggest its use as the off-the-shelf approach. Figures 20 and 21 in Appendix E depict the results for kNN. In EXPERT models, the second kNN pick tends to beat the task-agnostic one – hurting the kNN hybrid outcomes. Overall, the hybrid linear approach consistently outperforms the one based on kNN.

5.4 FURTHER ABLATION STUDIES

How does the computational budget impact the findings? We have seen that for a limited budget of B=2 the proposed hybrid method outperforms the other strategies. A natural question that follows is: how do these methods perform as a function of the computational budget B? In particular, for each budget B, we compute how frequently does a strategy pick the best model. The results are shown in Figure 6. We observe that the hybrid linear strategy outperforms all individual strategies on the ALL pool. Furthermore, it also outperforms a strong impractical task-agnostic oracle which is allowed to rank the models by the average fine-tune accuracy over all datasets. Our hybrid strategy achieves an on par performance with the linear approach on pools on which linear performs well. When task-aware strategies perform badly (e.g. pools without expert models), hybrid linear is significantly stronger (cf. Figure 16 in Appendix D). These empirical results demonstrate that the hybrid strategy is a simple yet effective practical choice.

Alternative evaluation scores. Both Meiseles & Rokach (2020) and Kornblith et al. (2019) compute the correlation between the ImageNet test accuracy and the average fine-tune accuracy across datasets. Although this provides a good task-agnostic evaluation method for the *average performance* (cf. Figure 1, right, in Kornblith et al. (2019)), it can be significantly impacted by outliers that have poor correlations on a specific dataset (cf. Figure 2, middle row, in Kornblith et al. (2019)). In Appendix B we highlight another limitation of using correlation scores in the context of model-search strategies across heterogeneous pools. Nevertheless, we empirically validate that ranking the models based on their ImageNet test accuracy on the IMNETACCURACIES pool transfers well to our evaluation setting (cf. Figure 13 in the Appendix D). Furthermore, we show that reporting the differences of logit-transformed accuracies (log-odds) leads to similar conclusions as ours (cf. Appendix C). We opt for the relative regret r(m), defined in Section 3, as it is more intuitive and contained in [-1,1].



Figure 6: **Optimal picks as a function of the computational budget.** The number of picked models (relative) with zero regret across three representative pools. We note that hybrid linear outperforms all other methods on ALL, whilst being comparable with the linear strategy on restricted pools where linear alone already performs well. Here, the task-agnostic oracle refers to a method which ranks models based on their average accuracy across all datasets (more details Section 5.4).

Impact of the kNN hyperparameters. The kNN classifier suffers from the curse of dimensionality (Snapp et al., 1991), which is why we study the impact of the dimension (i.e. the representation size) on the kNN evaluation. We fix a dataset, and plot a model's kNN score versus its representation dimension. In order to have a single point per dimension and avoid an over-representation of the expert models that are all of the same architecture, we choose the model with the best kNN accuracy. By calculating the Pearson correlation coefficient between the dimension and the respective kNN scores, we observe a moderate anti-correlation (R < -0.5) for 3 datasets, a moderate correlation (R > 0.5) for 3 other datasets, and either small or no correlation for the remaining 13 datasets. Based on this empirical evidence we conclude that there is no significant correlation between the kNN classifier accuracy and the dimension. We provide more details in Figure 22 of Appendix F. Regarding k, our preliminary experiments with k = 3 offered no significant advantages over k = 1.

6 CONCLUSIONS, LIMITATIONS, AND FUTURE WORK

Transfer learning offers a data-efficient solution to train models for a range of downstream tasks. As we witness an increasing number of models becoming available in repositories such as TensorFlow Hub, though, finding the right pre-trained models for target tasks is getting harder. Fine-tuning all of them is not an option. In practice, the computational budget is limited and efficient model search strategies become paramount. We motivate and formalize the problem of efficient model search through a notion of *regret*, and argue that regret is better suited to evaluate search algorithms than correlation-based metrics. Empirical evaluation results for the predominant strategies, namely *task-agnostic* and *task-aware* search strategies, are presented across several scenarios, showing that both can sometimes yield high regret. For any individual method we study, there exists a pool of models on which the method fails. Finally, we propose a simple and computationally efficient hybrid search strategy which consistently outperforms the existing approaches over 19 diverse vision tasks and across all the defined model pools.

Limitations and future work. To further stress-test the generalization of analysed strategies, the number of relevant model pools could be increased by incorporating more diverse upstream tasks, in particular neural architectures, losses, and datasets. This would potentially yield more expert models making the task even more challenging, and it could further highlight the advantages of an effective search strategy. Secondly, we observe that task-aware methods consistently perform poorly in specific cases, such as when we consider diverse architectures trained only on ImageNet. There is no obvious reason for such failures. Similarly, there seems to be a clear pattern where task-aware methods perform significantly worse on structured datasets than on natural ones. We hypothesise that this is due to the lack of adequate expert models for these domains. However, an in-depth analysis of these specific cases might be beneficial and insightful. Finally, transfer learning is a successful strategy in various natural language processing tasks, which we did not explore here due to the lack of diverse sources of text representation and heterogeneous pools in online repositories. Nevertheless, going beyond vision tasks presents a very clear research direction.

REFERENCES

- Jeff Donahue, Yangqing Jia, Oriol Vinyals, Judy Hoffman, Ning Zhang, Eric Tzeng, and Trevor Darrell. Decaf: A deep convolutional activation feature for generic visual recognition. *International Conference on Machine Learning*, 2014.
- Eyal Even-Dar, Shie Mannor, and Yishay Mansour. Action elimination and stopping conditions for the multi-armed bandit and reinforcement learning problems. *Journal of Machine Learning Research*, 2006.
- Weifeng Ge and Yizhou Yu. Borrowing treasures from the wealthy: Deep transfer learning through selective joint fine-tuning. *IEEE Conference on Computer Vision and Pattern Recognition*, 2017.
- Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. Deep residual learning for image recognition. *IEEE Conference on Computer Vision and Pattern Recognition*, 2016.
- Kaiming He, Ross Girshick, and Piotr Dollár. Rethinking imagenet pre-training. *IEEE Conference on Computer Vision and Pattern Recognition*, 2019.
- Andrew G Howard, Menglong Zhu, Bo Chen, Dmitry Kalenichenko, Weijun Wang, Tobias Weyand, Marco Andreetto, and Hartwig Adam. Mobilenets: Efficient convolutional neural networks for mobile vision applications. *arXiv preprint arXiv:1704.04861*, 2017.
- Minyoung Huh, Pulkit Agrawal, and Alexei A Efros. What makes ImageNet good for transfer learning? *arXiv preprint arXiv:1608.08614*, 2016.
- Alexander Kolesnikov, Xiaohua Zhai, and Lucas Beyer. Revisiting self-supervised visual representation learning. *IEEE Conference on Computer Vision and Pattern Recognition*, 2019.
- Simon Kornblith, Jonathon Shlens, and Quoc V Le. Do better Imagenet models transfer better? *IEEE Conference on Computer Vision and Pattern Recognition*, 2019.
- Chenxi Liu, Barret Zoph, Maxim Neumann, Jonathon Shlens, Wei Hua, Li-Jia Li, Li Fei-Fei, Alan Yuille, Jonathan Huang, and Kevin Murphy. Progressive neural architecture search. *European Conference on Computer Vision*, 2018.
- Amiel Meiseles and Lior Rokach. Source model selection for deep learning in the time series domain. *IEEE Access*, 2020.
- Jiquan Ngiam, Daiyi Peng, Vijay Vasudevan, Simon Kornblith, Quoc V Le, and Ruoming Pang. Domain adaptive transfer learning with specialist models. *arXiv preprint arXiv:1811.07056*, 2018.
- Maxime Oquab, Leon Bottou, Ivan Laptev, and Josef Sivic. Learning and transferring mid-level image representations using convolutional neural networks. *IEEE Conference on Computer Vision and Pattern Recognition*, 2014.
- Sinno Jialin Pan and Qiang Yang. A survey on transfer learning. *IEEE Transactions on Knowledge and Data Engineering*, 2009.
- Joan Puigcerver, Carlos Riquelme, Basil Mustafa, Cedric Renggli, André Susano Pinto, Sylvain Gelly, Daniel Keysers, and Neil Houlsby. Scalable transfer learning with expert models. *arXiv* preprint arXiv:1910.04867, 2020.
- Olga Russakovsky, Jia Deng, Hao Su, Jonathan Krause, Sanjeev Satheesh, Sean Ma, Zhiheng Huang, Andrej Karpathy, Aditya Khosla, Michael Bernstein, et al. Imagenet large scale visual recognition challenge. *International Journal of Computer Vision*, 2015.
- Ali Sharif Razavian, Hossein Azizpour, Josephine Sullivan, and Stefan Carlsson. CNN features off-the-shelf: An astounding baseline for recognition. *IEEE Conference on Computer Vision and Pattern Recognition*, 2014.
- Robert R Snapp, Demetri Psaltis, and Santosh S Venkatesh. Asymptotic slowing down of the nearest-neighbor classifier. *Advances in Neural Information Processing Systems*, 1991.

- Christian Szegedy, Vincent Vanhoucke, Sergey Ioffe, Jon Shlens, and Zbigniew Wojna. Rethinking the Inception architecture for computer vision. *IEEE Conference on Computer Vision and Pattern Recognition*, 2016.
- Chuanqi Tan, Fuchun Sun, Tao Kong, Wenchang Zhang, Chao Yang, and Chunfang Liu. A survey on deep transfer learning. *International Conference on Artificial Neural Networks*, 2018.
- Zirui Wang. Theoretical guarantees of transfer learning. arXiv preprint arXiv:1810.05986, 2018.
- Karl Weiss, Taghi M Khoshgoftaar, and DingDing Wang. A survey of transfer learning. *Journal of Big data*, 2016.
- Xiaohua Zhai, Joan Puigcerver, Alexander Kolesnikov, Pierre Ruyssen, Carlos Riquelme, Mario Lucic, Josip Djolonga, Andre Susano Pinto, Maxim Neumann, Alexey Dosovitskiy, et al. The Visual Task Adaptation Benchmark. *arXiv preprint arXiv:1910.04867*, 2019.
- Barret Zoph, Vijay Vasudevan, Jonathon Shlens, and Quoc V Le. Learning transferable architectures for scalable image recognition. *IEEE Conference on Computer Vision and Pattern Recognition*, 2018.

A PRE-TRAINED MODEL DETAILS

We provide a detailed list of all the used pre-trained models together with the dimension of their representations, the number of parameters, and the achieved ImageNet test accuracy (for those that the accuracy is known), in the following tables.

Table 1: ImageNet Classification Models – All models are accessible by using the same prefix "https://tfhub.dev/google/imagenet/" in front of the model name.

Model Name	Dim	# Params	ImageNet Accuracy
inception_v1/feature_vector/4	1024	5'592'624	0.698
inception_v2/feature_vector/4	1024	10'153'336	0.739
inception_v3/feature_vector/4	2048	21'768'352	0.78
inception_resnet_v2/feature_vector/4	1536	54'276'192	0.804
resnet_v1_50/feature_vector/4	2048	23'508'032	0.752
resnet_v1_101/feature_vector/4	2048	42'500'160	0.764
resnet_v1_152/feature_vector/4	2048	58'143'808	0.768
resnet_v2_50/feature_vector/4	2048	23'519'360	0.756
resnet_v2_101/feature_vector/4	2048	42'528'896	0.77
resnet_v2_152/feature_vector/4	2048	58'187'904	0.778
mobilenet_v1_100_224/feature_vector/4	1024	3'206'976	0.709
mobilenet_v2_100_224/feature_vector/4	1280	2'223'872	0.718
nasnet_mobile/feature_vector/4	1056	4'232'978	0.74
nasnet_large/feature_vector/4	4032	84'720'150	0.827
pnasnet_large/feature_vector/4	4320	81'736'668	0.829

Table 2: Expert Models – The model name indicates the subset of JFT on which each model was trained (Puigcerver et al., 2020).

Model (Subset)	Dim	# Params
Mode of transport	2048	23'807'702
Geographical feature	2048	23'807'702
Structure	2048	23'807'702
Mammal	2048	23'807'702
Plant	2048	23'807'702
Material	2048	23'807'702
Home & garden	2048	23'807'702
Flowering plant	2048	23'807'702
Sports equipment	2048	23'807'702
Dish	2048	23'807'702
Textile	2048	23'807'702
Shoe	2048	23'807'702
Bag	2048	23'807'702
Paper	2048	23'807'702
Snow	2048	23'807'702
Full JFT	2048	23'807'702

Table 3: VTAB Benchmark Models – All models are accessible by using the model name and the prefix "https://tfhub.dev/vtab/".

Model Name	Dim	# Params
sup-100/1	2048	23'500'352
rotation/1	2048	23'500'352
exemplar/1	2048	23'500'352
relative-patch-location/1	2048	23'500'352
jigsaw/1	2048	23'500'352
semi-rotation-10/1	2048	23'500'352
sup-rotation-100/1	2048	23'500'352
semi-exemplar-10/1	2048	23'500'352
sup-exemplar-100/1	2048	23'500'352
cond-biggan/1	1536	86'444'833
uncond-biggan/1	1536	86'444'833
wae-mmd/1	128	23'779'136
wae-gan/1	128	23'779'136
wae-ukl/1	128	23'779'136
vae/1	128	23'779'136

B LIMITATION OF CORRELATION AS EVALUATION SCORE

Previous works follow an approach that performs a correlation analysis on choosing which model to transfer based on a ranking across the models (Kornblith et al., 2019; Meiseles & Rokach, 2020). We claim that this is not a suitable score in our setting of heterogenous pools, and in this section we explain the arguments in more details. We provide a simple example in which a correlation analysis fails compared to our notion of regret, which we see as an intuitive notion of failure in this setting.

We start by outlining two obvious dependencies between the two variants:

- Having a perfect correlation (equal to 1) results in zero regret,
- Having zero regret does not necessarily imply a perfect correlation.

The first statement follows by definition, whereas the second statement is justified by the following example: suppose that all models perform identically in terms of the fine-tune accuracy. In this case, every attribute (e.g. proxy task value, or ImageNet accuracy) would yield no correlation with respect to the fine-tune accuracy, although there is clearly zero regret for every imaginable strategy.

Implications. If we have a large pool of models with some outlier models that clearly outperform the others, which are of similar fine-tune accuracy, a search strategy should return one of those *better* model, otherwise it will suffer from a large regret. On the other hand, this setting would usually have no rank nor linear correlation following the reasoning from before. If we restrict the same pool to models performing similarly, it will remain uncorrelated, but every search strategy will result in zero regret. The same scenario holds if single outliers are performing worse than all other models. Both cases are seen often in practice, especially for model pools containing experts. We highlight some examples of this phenomena in Figures 7 and 8, together with some that have positive correlation.

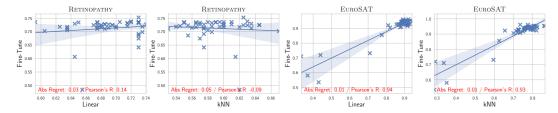


Figure 7: Example correlation values for pool ALL.

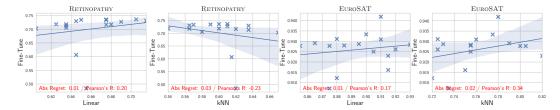


Figure 8: Example correlation values for pool EXPERT.

C LOG-ODDS FOR THE EVALUATION SCORE

Following Kornblith et al. (2019), we analyze a notion that differs from our definition of relative regret and delta between two strategies (cf. Equation 2 and Section 3). The idea is to compare two search strategies m_1 and m_2 by calculating the difference between $\operatorname{logit}(s(m_1))$ and $\operatorname{logit}(s(m_2))$ (the expected maximal logit-transformed test accuracy achieved by any model in the sets returned for both search strategies). The logit transform is defined as $\operatorname{logit}(p) = \operatorname{log}(p/(1-p)) = \operatorname{sigmoid}^{-1}(p)$, also known as the log-odds of p. This transformation leads to the next definition of $\operatorname{log-odds}$ delta:

$$\tilde{\Delta}(m_1, m_2) := \log \left(\frac{s(m_1) - s(m_2)}{1 - \min(s(m_1), s(m_2))} \right). \tag{3}$$

Substituting $s(m_1)$ by the ORACLE value from Equation 1 in Section 3, and $s(m_2)$ by s(m) leads to a new definition of log-odds regret $\tilde{r}(m)$.

These definitions are also incorporating the dataset difficulty and yield results very similar to our definition of the relative delta and relative regret in Section 3. We now provide the analogous plots of the ones given in the main body of the paper, with the log-odds regret and log-odds delta instead of the relative regret and relative delta. We highlight the fact that, beside the change of the scale on the y-axis, all the findings given in the main body of the paper hold.

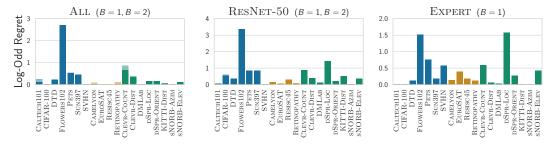


Figure 9: Log-odds regret $(\tilde{r}(m))$ with B=1 (transparent) and B=2 (solid) for the task-agnostic model search strategy.

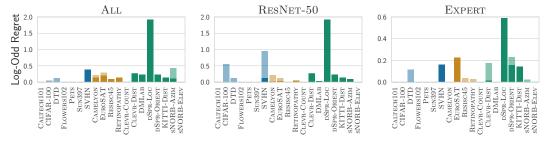


Figure 10: Log-odds regret $(\tilde{r}(m))$ for B=1 (transparent) and B=2 (solid) for the task-aware (linear) model search strategy.

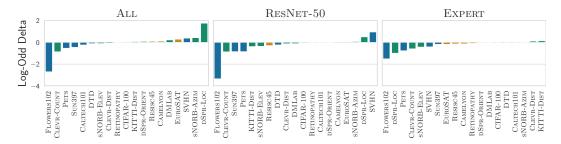


Figure 11: Log-odds delta $(\tilde{\Delta}(m_1, m_2))$ between task-agnostic (positive if better) and Task-aware (linear) (negative if better) for B=1.

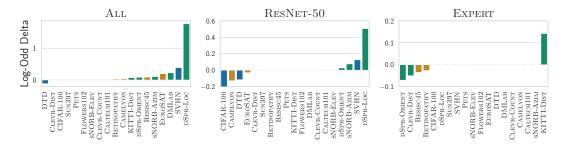


Figure 12: Log-odds delta $(\tilde{\Delta}(m_1, m_2))$ between hybrid linear (positive if better) and linear evaluation (negative if better) for B=2.

D ANALYSIS FOR OTHER POOLS.

In this sections we provide the plots and an analysis for the DIM2048 and IMNETACCURACIES pools, both omitted from the main body of the paper.

We start by emphasizing that the results between the DIM2048 and the RESNET-50 pool, used in the main body of the paper, do not vary significantly. Most notably, the hybrid linear strategy is on par with the task-aware method, whereas the task-agnostic method suffers from high regret due to the lack of ability to pick expert models.

When examining the performance of all strategies on the IMNETACCURACIES pool, presented in Figure 13 (right), Figure 14 (right) and Figure 15 (right), we observe that the task-agnostic strategy is able to pick the optimal model for 12 out of 19 datasets for B=1, and as many as 17 out of 19 for B=2. This clearly confirms the claim made by Kornblith et al. (2019) that better ImageNet models transfer better. More surprisingly, we observe that both task-aware strategies (linear and kNN) fail consistently and, hence, result in high regret when being restricted to the IMNETACCURACIES pool only (cf. Figures 14 and 15).

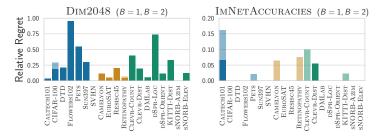


Figure 13: Relative regret for the task-agnostic search strategy with B=1 (transparent) and B=2 (solid) on the pools DIM2048 and IMNETACCURACIES.

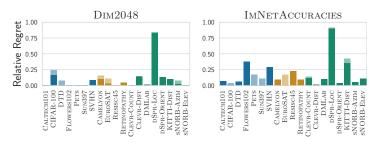


Figure 14: Relative regret for the task-aware (linear) search strategy with B=1 (transparent) and B=2 (solid) on the pools DIM2048 and IMNETACCURACIES.

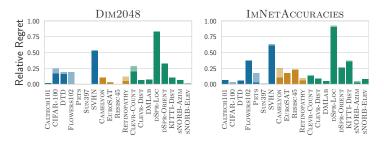


Figure 15: Relative regret for the task-aware (kNN) search strategy with B=1 (transparent) and B=2 (solid) on the pools DIM2048 and IMNETACCURACIES.



Figure 16: Optimal picks for an increasing budget on DIM2048 and IMNETACCURACIES.

E kNN as a task-aware proxy

In this section, we analyze the impact of choosing the kNN classifier accuracy as the choice for the proxy task, compared to the linear classifier accuracy described in the main body of the paper. In practice, kNN might be favorable to a user since calculating the kNN classifier accuracy with respect to a relatively small test set can be orders of magnitude faster compared to training a linear classifier, which might be sensitive to the choice of optimal hyper-parameters. A theoretical and empirical analysis of the computing performance of these two proxies is out of the scope of this work, as we are mainly interested in the comparison in terms of the model-search capability of either of these. In general, the major claims on the performance of linear as a task-aware strategy also apply to kNN. The latter also mainly fails on structured datasets across all pools, as visible in Figure 17. Similarly to the linear task, kNN is on par with the task-agnostic strategy on the ALL pool, but clearly outperforms it on the RESNET-50 and EXPERT pools, as visible in Figure 18. By further comparing kNN to the linear proxy task, we realize that kNN performs worse than linear on half of the datasets across the three different dataset groups, whilst being on par with it on the other half (cf. Figure 19). Finally, by choosing kNN as the task-aware part for the hybrid strategy and comparing it to the task-aware (kNN) strategy with a budget of B=2 in Figure 20, we see an increase of performance on the ALL pool, no clear winner on the restricted RESNET-50 pool, but higher regret on the EXPERT pool. Unsurprisingly, this version of hybrid strategy also performs slightly worse compared than the one with a linear proxy across all the pools (cf. Figure 21).

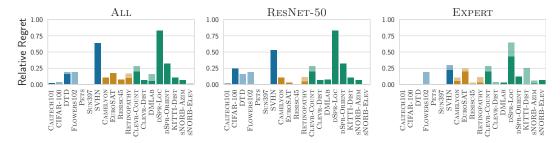


Figure 17: Relative regret for the kNN search strategy with B=1 (transparent) and B=2 (solid).

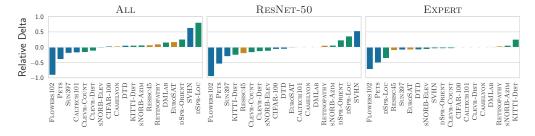


Figure 18: Relative delta between the task-agnostic (positive if better) and the kNN task-aware search strategy (negative if better) for B=1.

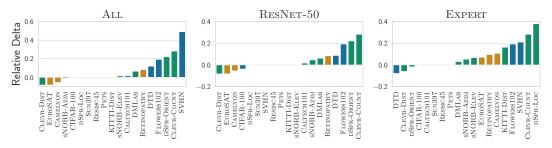


Figure 19: Relative delta between the linear (positive if better) and the kNN task-aware search strategy (negative if better) for B=1.

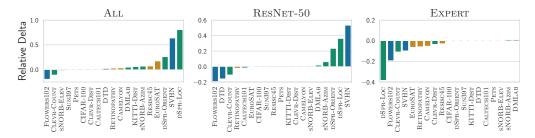


Figure 20: Relative delta between the hybrid kNN (positive if better) and kNN search strategy (negative if better) for B=2.

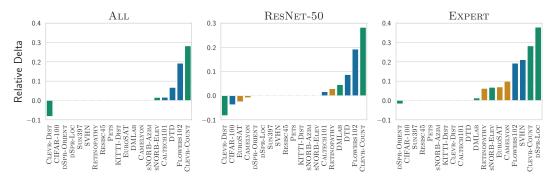


Figure 21: Relative delta between the hybrid Linear (positive if better) and hybrid kNN search strategy (negative if better) for B=2.

F ON THE IMPACT OF THE DIMENSION ON kNN

As described in Section 5.4, in this section we show that there is no signification correlation (positive or negative) between the kNN classifier accuracy and the dimension of the representation that it is evaluated on. We see this by running a linear correlation analysis between the dimension of the each representation and the achieved kNN classifier accuracy. In order to have a single point for each possible dimension, and to avoid an over-representation of the expert models, which have all the same dimension, for each dimension we selected the model that achieves the highest kNN accuracy. We do this for all pairs of dimensions and datasets. In Figure 22 we present three hand-picked datasets that achieve (a) the highest anti-correlation value, (b) the lowest absolute correlation value, and (c) the highest correlation value.

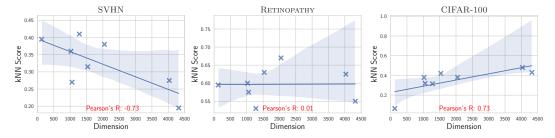


Figure 22: Three examples of datasets in which the analysis of the dimension of the representation compared to the resulting kNN scores results in a negative correlation (**left**), no correlation at all (**middle**), and a positive correlation (**right**).

G BUDGET PER METHOD

In this section, we display the budget each method requires in order to achieve zero regret per pool. Notice that the strategy "Oracle" refers to the task-agnostic oracle which ranks models based on their achieved average accuracy over all datasets. Even though this is not practical, it enables us to have a task-agnostic method that is able to achieve zero regret eventually as every model (even experts) is included in this ranking. We split the results by the dataset types and notice that there are some clear patterns between a pool, a dataset type and the required budget for task-aware or task-agnostic methods. For instance, one observes that the linear strategy performs well on all the natural datasets across all the pools except IMNETACCURACIES. Structured and specialized datasets seem to be harder for this proxy task, except for the EXPERT pool. Finally, kNN consistently performs slightly worse than the linear proxy across all pools.

Table 4: Budget required to achieve zero regret per datataset and strategy on the pools ALL, RESNET-50 and EXPERT.

		ALL		RESNET-50			Expert		
Dataset	Oracle	Linear	kNN	Oracle	Linear	kNN	Oracle	Linear	kNN
CALTECH101	5	1	4	3	1	2	1	1	1
CIFAR-100 ●	1	2	2	1	2	6	1	1	1
DTD •	9	2	3	6	2	2	3	2	1
FLOWERS 102	26	1	2	20	1	2	11	1	2
Pets •	13	1	1	9	1	1	5	1	1
Sun397 •	7	1	1	5	1	1	2	1	1
SVHN •	1	23	37	2	9	13	15	13	15
CAMELYON •	23	5	9	17	4	8	9	1	4
EuroSAT •	1	4	19	14	16	7	4	5	5
RESISC45	1	35	34	3	1	1	2	2	2
RETINOPATHY •	2	4	8	23	14	9	12	2	7
CLEVR-COUNT •	7	1	10	5	1	9	2	1	6
CLEVR-DIST •	44	5	4	35	5	4	10	6	2
DMLab •	1	18	29	3	8	4	7	1	6
DSPR-LOC •	9	25	21	6	19	17	3	3	4
DSPR-ORIENT	30	9	21	23	8	19	12	5	12
KITTI-DIST •	3	8	14	1	7	10	1	3	2
sNORB-Azim •	1	45	25	32	3	5	1	2	15
sNORB-ELEV •	37	1	2	30	1	1	12	1	5

Table 5: Budget required to achieve zero regret per datataset and strategy on the pools DIM2048 and IMNETACCURACIES.

	Г	ОІМ2048		IMNET	ACCURAC	TES
Dataset	Oracle	Linear	kNN	Oracle	Linear	ILS
CALTECH101	3	1	4	3	7	12
CIFAR-100 ●	1	5	10	1	2	2
DTD •	7	2	3	2	7	9
FLOWERS 102	24	1	2	1	14	15
Pets •	11	1	1	2	2	3
Sun397 •	5	1	1	1	2	2
SVHN •	2	12	15	1	14	15
CAMELYON •	21	5	9	2	7	8
EuroSAT •	17	21	8	1	2	8
RESISC45	3	1	1	1	14	14
RETINOPATHY •	6	12	6	2	3	4
CLEVR-COUNT •	5	1	10	2	12	12
CLEVR-DIST •	42	5	4	14	6	4
DMLab •	9	10	8	1	9	12
DSPR-LOC •	7	25	21	1	15	13
DSPR-ORIENT	28	9	21	1	8	12
KITTI-DIST •	1	8	13	2	13	15
sNORB-Azim	37	4	7	1	14	9
sNORB-ELEV •	35	1	2	1	15	15

H ALL FINE-TUNE ACCURACIES AND PICKED MODELS

Finally, we provide plots that summarize all the results of the conducted large-scale experiment in a single overview per pool. The plots highlight the range of test accuracies amongst all the fine-tuned models, as well as the returned top-1 models (B=1) for the three strategies – task-agnostic, task-aware linear and task-aware $k{\rm NN}$.

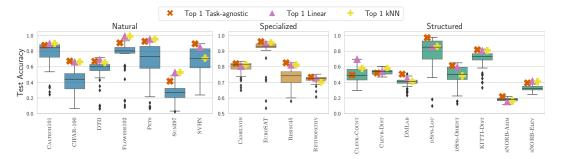


Figure 23: Pool ALL.

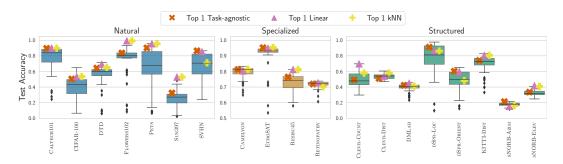


Figure 24: Pool DIM2048.

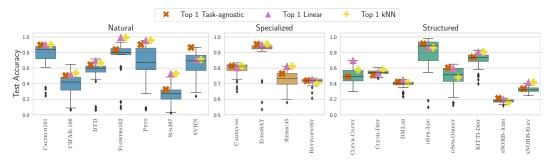


Figure 25: Pool RESNET-50.

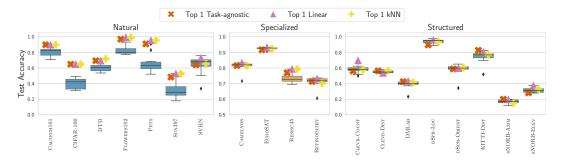


Figure 26: Pool EXPERT.

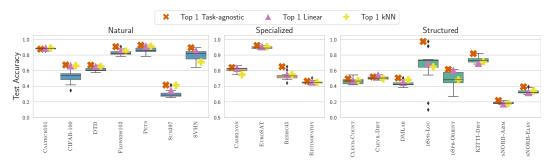


Figure 27: Pool IMNETACCURACIES.