Occam's Razor for Self Supervised Learning: What is Sufficient to Learn Good Representations?

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Abstract

Recent Self Supervised Learning (SSL) solutions have introduced numerous additional design choices, e.g., a projector network, positive views, or teacher-student networks. These additions limit the impact of theoretical studies that often fail to incorporate all those intertwined designs and slow-down the deployment of SSL methods to new domains as numerous hyper-parameters need to be carefully tuned. In this study, we demonstrate that for pretraining datasets of up to a few hundred thousands samples—the additional designs introduced by SSL can be removed without negatively impacting performances. That finding should tremendously simplify the practitioner's path to SSL deployment in numerous small and medium scale settings. In addition, our finding answers a long-lasting question: the oftenexperienced sensitivity to training settings and hyper-parameters encountered in SSL come from their design, rather than the absence of supervised guidance–as our simplified method is robust to changes in hyper-parameters and datasets.

1 Introduction

Self-Supervised Learning (SSL) [1, 2] has recently demonstrated that one can train, without labels, highly non-trivial Deep Neural Networks (DNNs) whose representations are often richer than supervised ones [3]. In particular, SSL differs from *reconstruction-based* methods such as (denoising,

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Algorithm	1 Our p	proposed	simplified	SSL	solution:	DIET
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# take any preferred DNN e.g. resnet50 # see Algorithm 2 for other examples $f = torchvision.models.resnet50() # f_{\theta}$ # f comes with a classifier so we remove it	from torch.utils.data import Dataset, DataLoader from torchvision.datasets import CIFAR100
K = f.fc.in_features f.fc = nn.ldentity()	class DatasetWithIndices(Dataset): definit(self, dataset):
# define DIET's linear classifier and XEnt W = nn.Linear(K, N, bias=False) # W in Eq. (1) XEnt = nn.CrossEntropyLoss(label_smoothing=0.8)	<pre>self.dataset = dataset defgetitem(self, n): # disregard the labels x, _ = self.dataset[n]</pre>
<pre># define dataset and train (Fig. 1) train_dataset = DatasetWithIndices(train_dataset) train_loader = DataLoader(train_dataset,)</pre>	return x, n deflen(self): return len(self.dataset)
for x, n in train_loader: loss = XEnt(W(f(x)), n)	<pre># example with CIFAR100 C100 = CIFAR100(root) C100_w_ind = DatasetWithIndices(C100)</pre>

variational, masked) Autoencoders [4, 5, 6] and their variants by removing the need for a *decoder* DNN and an input-space reconstruction loss, both being difficult to design [7, 8, 9, 10]. Nonetheless, SSL which is the current state-of-the-art unsupervised learning solution, comes with many moving pieces, for instance, a carefully designed *projector* DNN g_{γ} to perform SSL training with the composition $g_{\gamma} \circ f_{\theta}$ and throwing away the projector (g_{γ}) afterwards [1], or advanced anti-collapse techniques involving moving average teacher models [11, 12], representation normalization [13, 14], or Entropy estimation [1, 15]. An incorrect pick of any of those moving pieces results in a drastic drop in performances [16, 17]. Most of those design choices have, however, been explored, carefully-tuned over many works, and set in stone when considering large scale natural images.

But how can one deploy such pipelines to new label-free data modalities when so many design choices need to be carefully tuned?

As of today, one would (i) either avoid learning altogether and use a pretrained model most commonly from Imagenet, or (ii) cross-validate again the many hyper-parameters of SSL models albeit requiring one to come up with some proxy to be used as validation metric. It is known that (i) can be highly suboptimal when considering non natural images such as medical [18], and (ii) is practically unrealistic without labels as SSL losses fail to convey any qualitative information about the representation being learned [19, 20]. From the above, we argue that **Self Supervised Learning Needs Occam's Razor**–and we provide additional background and arguments in Appendix A.

To alleviate those limitations, we propose a stripped-down SSL method-coined DIET-that enables one to perform SSL on small to medium scale dataset without requiring labels. In fact, DIET is not sensitive to its (few) hyper-parameters and thus can be used as-is across data modalities, architectures, optimizers, ... In addition, the DIET's loss value is also a strong indicator of quality of the representation. Hence, label-free evaluation is also made possible. We summarize below the key benefits of DIET:

- 1. **Competitive on common benchmarks and SOTA on medical and small datasets:** on more than 13 datasets including natural images (Table 1) and medical images (Section 3.2) even against SSL benchmarks pretrained on Imagenet (Table 5).
- 2. **Stable and Out-of-the-box:** consistently high performances without hyper-parameter tuning as tested across 16 architectures including ConvNexts, ViTs, 13 datasets, models, optimizers(Tables 1, 3 and 5).
- 3. **Practical, Efficient, and theory-friendly:** from the absence of positive pairs, projector networks, and decoders DIET training requires same resources as supervised learning. All our experiments are done on a single GPU. We also find DIET's training loss to strongly correlate with the downstream task test accuracy across architectures and datasets (Fig. 3).

An interactive demo is provided in this colab notebook.

2 DIET: Occam's Razor for Stable Small to Medium Scale SSL

The goal of this section is to introduce the proposed objective (Eq. (1)) that we will use to contrast with current SSL objectives. Thorough empirical validations on natural and medical images are provided in the next Sections 3.1 and 3.2

Simplification 1: from relative to absolute loss. Self Supervised Learning compares the intersample representations, aiming to *collapse* together the positive pairs, while ensuring that the entire representation does not collapse [21, 22, 23]. Within that formulation, SSL treats each sample and its views as a single class. We thus replace the relative inter-sample objective with a cross-entropy loss using as target the index of the original datum. That is, given a dataset of N samples $\{x_1, \ldots, x_N\}$, define the class of sample x_n with $n \in \{1, \ldots, N\}$ to be n itself.

Simplification 2: removal of the nonlinear projector. We remove the usual nonlinear projector (g_{γ}) and instead only use a liner classifier that maps the K-dimensional output of the originally considered model f_{θ} to the N classes of the cross-entropy objective. We denote that linear classifier as $\boldsymbol{W} \in \mathbb{R}^{N \times K}$,

Simplification 3: removal of teacher-student network and positive pairs. Additionally, we remove the need to have positive pairs and teacher-student network as the XEnt already prevents collapse and W "memorize" the class centroids, i.e., other positive views.

Table 1: **DIET often outperforms benchmarks on CIFAR100.** We employ the settings of Fig. 6, notice the consistent progression of the performance through architectures which is not easily achieved with standard SSL methods without per-architecture cross-validation. Benchmarks taken from \dagger :[27]; \ddagger :[28]; \ast :[29]; \bullet :[30]; \diamond :[31]; \star :[32]; \triangleleft :[33]; \triangleright :[34]; \Box :[35],1:[36], 2 :[37], IN100 provided in Table 4. **CIFAR100**

		Resnet50							
Resnet18		MoCoV2	53.44*			Time	agamat		
SimCLR	57.81 [▷]	SimMoCo	54.64*	TinyImagenet					
DINO	58.12 [•]	SimCO	58.48*		iet18				
SimCO	58.35*	SimCLR	61.10*	SimSiam	44.5	4 [‡]	Resi	iet50	
SimCLR+DCL	58.50 [†]	SimCLR+DCL	62.20*	SimCLR	46.2	1 [‡]	SimCLR	48.1	2^{2}
SimCLR	60.30 [‡]	MoCoV3	69.00 [⊲]	BYOL	47.2	3‡	SimSiam	46.7	
SimCLR	60.45°	DIET	69.91	MoCo	47.9	-	Spectral	49.8	
W-MSE	61.33	Resnet101							
SimCLR+CC	61.91 [‡]	SimCLR	52.28	SimCLR	48.7		CorInfoMax	34.8	0
BYOL	62.01	SimCLR+adv	59.02 [†]	DINO	49.2				
MoCoV2	62.34	MoCoV3	68.50⊲			DI			
BYOL	63.75 [‡]	DIET	71.39	resnet18		45.07	MLPMixer		39.32
DIET	63.77	AlexNet		resnet34		47.04	vit_b_16		48.38
BYOL+CC	64.62 [‡]	SplitBrain	39.00□	wide_resnet	50_2	50.03	densenet121		49.38
SimSiam	64.79 [‡]		39.40□	resnet50		51.66	convnext_sn	ıall	50.05
	64.79°	DeepCluster	41.90 [□]	resnet101		51.86	swin_t		50.80
SwAV SimCLR	65.78°	AND	47.90	resnext50_3	2x4d	52.45	convnext_tir	ıy	50.88
		DIET	47.90						
SimSiam+CC	65.82 [‡]								
		SeLa	57.40□						

Leading to the final formulation

$$\mathcal{L}_{\text{DIET}}(\boldsymbol{x}_n) = \text{XEnt}(\boldsymbol{W} \boldsymbol{f}_{\boldsymbol{\theta}}(\boldsymbol{x}_n), n), \tag{1}$$

given a sample $x_n \in \mathbb{R}^D$. We highlight that we couldn't find an existing study that proposed and experiment with Eq. (1). However, some close variations exist such as *Exemplar CNN* [24],*Instance Discrimination* [25] or *Noise as Targets* [26] which we discuss in Appendix C.

3 DIET: Stable Self Supervised Learning for any Modality and Model

To support the different claims we have made in the previous section, we will first explore natural image datasets in Section 3.1 and then move to medical images in Section 3.2 Throughout our study we rigorously follow the experimental setup described in Fig. 6 to demonstrate the stability of DIET, more specialized design choices should naturally lead to greater performance, if desired. Thorough ablation studies showing how DIET's performance are minimally impacted by optimizers, batch size, and other hyper-parameter changes are provided in Appendix D.

3.1 On Natural Images Against SSL With and Without Imagenet Pretraining

DIET achieves high performance on CIFAR100: Let's first consider CIFAR100 [38] with a few variations of Resnet [39] and AlexNet [40] architectures. On Alexnet, a few non-SSL baselines are available: SplitBrain [41], DeepCluster [42], InstDisc [25], AND [43], SeLa [44], and ReSSL [45]. Our models are trained with the DIET objective (Eq. (1)), and linear evaluation is employed to judge the quality of the learned representation. We report results Table 1 where we observe that DIET is able to match and often slightly exceed current SSL methods. Also, increasing the DNN capacity, *i.e.*, from Resnet18 to Resnet101 does not exhibit any overfitting using DIET.

DIET achieves high performance on TinyImagenet and IN00: We broaden the considered space of architectures to not only include the Resnet variants, but also SwinTransformers [46], VisionTransforms [47], Densenets [48], ConvNexts [49], WideResnets [50], ResNexts [51], and the MLPMixer [52]. We report those results in Table 1 where we observe that DIET is now around the average performance of the multiple SSL methods combined. As most SSL methods have been thoroughly tuned for Imagenet style tasks, we expect those benchmarks to be more challenging. That being said, the results from Table 1 demonstrate how DIET handles out-of-the-box any architecture change–even for different architecture families, e.g., with and without self-attention.

DIET trained on small datasets competes with Imagenet pre-trained SSL. We consider small datasets that are commonly handled by SSL through transfer learning: Aircraft [53], DTD [54], Pets [55], Flowers [56], CUB200 [57], Food101 [58], Cars [59]. By contrast, DIET finally provides an

dataset	bloodmnist	dermamnist]	pathmnist
DIET DIET+	89.24 90.44	73.92 74.21	44.53 44.54
MoCov2	53.70	66.88	18.97
SimCLR VICReg	14.56 47.18	66.88 66.78	$11.80 \\ 11.31$
Transfer	88.13	74.06	59.37

Table 2: Performance on MedMNIST datasets using a Resnet18 (ViT provided in Table 8). DIET+ refers to the same DIET model trained for the same number of GPU hours as other models. VICReg is trained with the same hyperparameters as SimCLR with SGD 6e-2. Transfer is pretrained on ImageNet and fixed with a linear probe.

alternative approach by training directly on the such small dataset. We report those results in Table 5 where we see that DIET competes with or in some cases outperforms SSL models pretrained on much larger dataset.

We also find DIET can even outperform supervised learning methods in some cases when few datalabels are available. Furthermore, we show DIET's learning objective can be used with specialized network architectures such as scattering networks. We refer interested reader to Appendix J for details of these explorations.

3.2 On Medical Images

We now propose a more challenging comparison on medical images–an important modality that is often left behind when developing and tuning new SSL methods. We will see that DIET is able to produce state-of-the-art performances out-of-the-box.

We evaluate DIET training from scratch on three datasets from the MedMNISTv2 benchmark [60] (i) PathMNIST consisting of 90,000 training images and 7,180 test images, (ii) DermaMNIST consisting of 10,015 training and 2,005 test images, and finally (iii) BloodMNIST consisting of 17,092 training and 3,421 test images. To match a realistic unsupervised representation learning scenario, we employ for each method the hyper-parameters that work well on CIFAR100, and assume no labels are available for SSL training. For DIET, we use the same hyperparameters used for CIFAR100. For the baseline SSL methods, we select a variety of methods including a contrastive method (SimCLR), a momentum based method (MoCov2), and a recent non-contrastive method (ViCReg). For those, we use the default hyperparameters from [61] which yield good performance (> 80%) on CIFAR10, a comparable small dataset consisting of 60,000 images.

We find that although all algorithms achieve high training accuracy via a linear probe as shown in Section 3.2, the features learned by the baseline SSL methods do not generalize well to the test sets. By contrast, DIET achieves much higher performances (also see Appendix K for DIET with ViT). We also show training curves for both the DIET loss and the online training accuracy which exhibit stable convergence out-of-the-box with the same hyper-parameters used throughout the paper in Fig. 10. In addition, DIET's simplicity makes it faster to reach a given number of epochs, specifically for ResNet18, DIET is 1.75x faster than SimCLR (and 1.72x faster than VICReg), thanks to DIET's simple learning objective.

4 Conclusions and Future Work

We examined current SSL pipelines and identified a few core components that clearly improve the quality of learned representations: (i) large number of training epochs, and (ii) strong and informed data augmentation. However, for numerous settings we explored, i.e., dataset with less than a few hundred thousands samples, the additional SSL complications, such as, positive views, nonlinear projector networks, teacher-student networks, do not help. On the contrary, we found that remove those additional parts of SSL pipelines make training much more stable and robust to changes in architecture, data modality, dataset size, and batch size. Even more surprising, the training objective now becomes informative of the downstream tasks test performance. We hope that our findings will help question which parts of our current pipelines are truly needed for case-by-case deployment, when knowing that they have been largely develop for large scale natural image tasks. Another impact of our findings lies the opening new doors to provable learning solutions. In fact, as the simpler pipeline we experimented with is easier to theoretically study, it could help in deriving novel and principled solutions.

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Supplementary Materials

The supplementary materials is providing the proofs of the main's paper formal results. We also provide as much background results and references as possible throughout to ensure that all the derivations are self-contained. Some of the below derivation do not belong to formal statements but are included to help the curious readers get additional insights into current SSL methods.

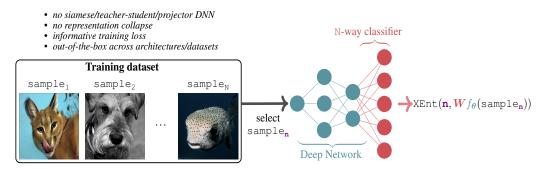


Figure 1: **DIET** uses the datum index (n) as the class-target –effectively turning unsupervised learning into a supervised learning problem. In our case, we employ the cross-entropy loss (X-Ent), no extra care needed to handle different dataset or architectures. As opposed to current SOTA, we do not rely on a projector nor positive views *i.e* no change needs to be done to any existing supervised pipeline to obtain DIET. As highlighted in Fig. 3, DIET's training loss is even informative of downstream test performances, and as ablated in Appendix D there is no degradation of performance with longer training, even for very small datasets (Table 5).

A Why Self Supervised Learning Needs Occam's Razor

Unsupervised learning often takes the form of intricate methods combining numerous moving pieces that need readjustment for each DNN architecture and dataset. As a result reproducibility, transferability across domains, and explainability are hindered.

Spectral embedding is computationally challenging. Spectral embedding takes many forms but can be summarized into estimating geodesic distances [62, 63] between all or some pairs of training samples to then learn a non-parametric [64, 65, 66, 67], or parametric [68, 69] mapping that produces embeddings whose pairwise distances matches the estimated geodesic ones. As such, spectral embedding heavily relies on the estimation of the geodesic distances which is a challenging problem [70, 71, 72], especially for images and videos [73, 74]. This limitation motivated the development of alternative methods, *e.g.*, Self-Supervised Learning (SSL) that often employ losses similar to spectral embedding [21, 22, 75] but manage to move away from geodesic distance estimation through the explicit generation of positive pairs, *i.e.*, that are close neighbors on the data manifold.

Self-Supervised Learning is over-specialized. Despite impressive performance and rigorous theoretical motivation, SSL development was mostly driven by industry driven research and thus entirely focused on large-scale natural images and sounds. In fact, SSL has evolved to a point where novel methods are architecture and dataset specific. A few challenges that limit SSL to be widely adopted are (i) loss values which are uninformative of the DNN's quality [20, 76], partly explained by the fact that SSL composes the DNN of interest f_{θ} with a projector DNN g_{γ} appended to it during training and discarded afterwards, (ii) too many per-loss and per-projector hyper-parameters whose impact on the DNN's performances are hard to control or predict [11, 77, 78], and (iii) lack of transferability of the hyper-parameters across datasets and architectures [79, 80]Lastly, SSL requires heavy code refactoring, e.g., it requires to generate positive pairs and forward them to siamese DNNs, sometimes with one DNN having parameters as the moving average of the other. This makes SSL implementation more costly than supervised learning often requiring distributed training and long training schedules that, effectively, reduce the accessibility and inclusivity of SSL research [81].

Reconstruction-based learning is unstable. Reconstruction without careful tuning of the loss has been known to be sub-optimal for long [82, 83] and new studies keep reminding us of that [84]. The

argument is simple, suppose one aims to minimize a reconstruction metric R for some input x

$$R(d_{\gamma}(e_n(\boldsymbol{x})), \boldsymbol{x}), \tag{2}$$

where e_{η} and d_{γ} are parametrized learnable encoder and decoder networks respectively; $e_{\eta}(x)$ is the representation of interest to be used after training. In practice, as soon as some noise ϵ is present in the data, *i.e.* we observe $x + \epsilon$ and not x, that noise ϵ must be encoded by e_{η} to minimize the loss from Eq. (2) unless one carefully designs R so that $R(x + \epsilon, x) = 0$. However, designing such a *noise invariant* R has been attempted for decades [8, 85, 86, 87, 88] and remains a challenging open problem. Hence, many solutions rely on learning R, e.g., in VAE-GANs [9] bringing even further instabilities and training challenges. Other alternatives carefully tweak R per dataset and architectures, e.g., to only compute the reconstruction loss on parts of the data as with BERT [89] or MAEs [90]. Lastly, the quality of the encoder representation depends on its architecture but also on the decoder [91, 92] making cross-validation more costly and unstable [93].

SSL is the family of method that have produced the most significant state-of-the-art solutions in recent years. Hence, it is the solution of choice that any practitioner hopes to deploy. As such, we propose to take a step towards understanding and alleviating the many practical challenges that would be up against through **DIET**–a stripped down SSL pipeline.

B Benefits for Practical Deployment and Theoretical Research

There are many direct benefit of the DIET's objective emerging from its simplicity. We highlight both a theoretical and a practical benefit.

Benefit for theoretical research and provable guarantees. First, DIET opens numerous avenues for theoretical research. This is in sharp contrast with the original SSL methods. In fact, current SSL lacks of theoretical guarantees as all existing studies have derived optimality conditions at the projector's output [21, 36, 94, 95, 96, 97, 98, 99] which is not the output of interest since the projector is thrown away after SSL training and the DNN's output and the projector's output greatly differ [1, 16, 17, 100]. As a further demonstration of DIET's theory-friendliness, we propose in Appendix E a theoretical study of DIET with a linear model f_{θ} , in which case we are able to prove that DIET performs a low-rank decomposition of the input data matrix and provably recovers the data's principal components. Again, that last result highlights how Eq. (1) greatly reduces the barrier to derive novel theoretical results and guarantee for SSL.

Benefits for practical development and deployment Second, the amount of code refactoring is minimal: there is no change required for the data loading pipelines as opposed to SSL which requires positive pairs, no need to specify teacher-student architectures, and no need to design a projector/predictor DNN. Second, DIET's implementation is not architecture specific as we validate on Resne(x)ts, ConvNe(x)ts, Vision Transformers and their variants. Furthermore, DIET does not introduce any additional hyper-parameters in addition to the ones already present in supervised learning–and because DIET's training loss is informative of test classification performances (Fig. 3)–it opens the door to truly label-free SSL.

C Relation Between DIET and Existing SSL

Despite DIET's simplicity, we could not find an existing method that considered it perhaps due to the common belief that dealing with hundreds of thousands of classes (N in Fig. 1, the training set size) would not produce successful training. As such, the closest method to ours is *Exemplar CNN* [24] which extracts a few patches from a given image dataset, and treats each of them as their own class; this way the number of classes is the number of extracted patches, which is made independent from N. A more recent method, *Instance Discrimination* [25] extends this by introducing inter-sample discrimination. However, they do so using a non-parametric softmax, *i.e.*, by defining a learnable bank of centroids to cluster training samples; for successful training those centroids must be regularized to prevent representation collapse. As we will compare in Table 1, DIET outperforms Instance Discrimination and Exemplar CNN while being simpler. Lastly, methods such as *Noise as Targets* [26] and DeepCluster [42] are quite far from DIET as (i) they perform clustering and use the datum's cluster as its class, *i.e.*, greatly reducing the dependency on N; and (ii) they perform clustering in the output space of the model f_{θ} being learned which brings multiple collapsed solutions that force those

Table 3: Ablation studies indicate that **DIET benefits from longer training and stronger data augmentation while being robust to architecture and batch-size changes**. We report top1 test accuracy on CIFAR100 with varying training epochs (**top left**), on TinyImagenet with varying DA pipelines (Algorithm 3), and on TinyImagenet with 3k training epochs and with varying batch-size (**bottom**) with learning rate $0.001 \frac{\text{bs}}{256}$; additional comparisons on MedMNIST Table 6.

, ,		0		200			-				
Epochs		100	-00					DA strength respect 18	$1 \\ 31.48$	2	3 13.88
resnet18 resnet50 resnet101	37.71	47.86	54.04	60.23	64.24	69.51	69.91	resnet34 resnet50	32.93 40.24	45.60 48.80	45.75

batch-size	8	16	32	64	128	256	512	1024
resnet18	32.9	37.9	42.7	43.4	43.3	43.7	43.7	42.6

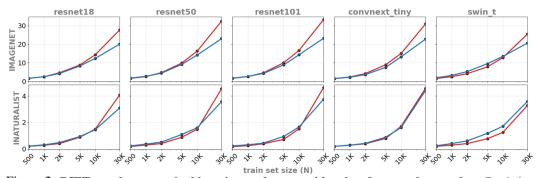


Figure 2: **DIET matches supervised learning on datasets with only a few samples per class.** Depiction of DIET's downstream performances (blue) against supervised learning (red) controlling training set size (**x**-**axis**); evaluation is performed over the original full evaluation set. DIET is able to learn highly competitive representations when the dataset is small with only a few samples per classes. See Fig. 7 for additional datasets.

methods to employ complicated mechanisms to ensure training to learn non-trivial representations. We note that while the added complexity enables those methods to scale to large datasets, it also greatly increases the performance sensitivity to the training hyper-parameters. We also emphasize in details why the simplifications put into DIET are crucial not only for deployment and theoretical guarantees in Appendices B and E.

D DIET's Dependency on Data-Augmentation, Training Time and Batch Size

The aim of this section is to better inform practitioners about the role of Data-Augmentations (DA), training time, and label smoothing in DIET's performances; as well as sensitivity to batch size, which is crucial for single-GPU training.

Batch-size does not impact DIET's performance. One important question when it comes to training a method with low resources is the ability to employ (very) small batch sizes. This is in fact one reason hindering the deployment of SSL methods which require quite large batch sizes to work (256 is a strict minimum in most cases). Therefore, we perform a small sensitivity analysis in Table 3 where we vary the batch size from 8 to 2048 without any hyper-parameter tuning other than the standard learning rate scaling used in supervised learning: $lr = 0.001 \frac{bs}{256}$. We observe small fluctuations of performances (due to a sub-optimal learning rate) but no significant drop in performance, even for batch size of 32. When going to 16 and 8, we observe slightly lower performances, likely due to batch-normalization [101] which is known to behave erratically below a batch size of 32 [102].

Data-Augmentation sensitivity is similar to SSL. We observed in the previous Section 3.1 that when using DA, DIET is able to perform on par with highly engineered state-of-the-art methods. Yet, knowing which DA to employ is not trivial, e.g., many data modalities have no obvious DA. One natural question is, thus, concerning the sensitivity of DIET's performance to the employed DA. To that end, we propose three DA regimes, one only consistent of random crops and horizontal flips (**strength:1**), which could be considered minimal in computer vision, one which adds color jittering and random grayscale (**strength:2**), and one last which further adds Gaussian blur and random erasing

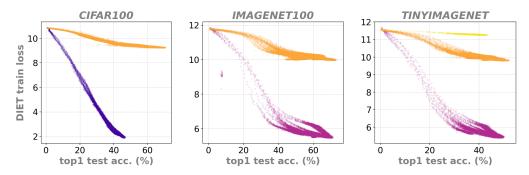


Figure 3: **DIET's training loss is indicative of downstream test performance.** We depict DIET's training loss (**y-axis**) against the online test linear probe accuracy (**x-axis**) for all the models, hyper-parameters, and training epochs. Yellow to purple correspond to different label smoothing which plays a role in DIET's convergence speed (Appendix D). For a given label smoothing parameter, there exists a strong relationship between **DIET**'s training loss and the downstream test accuracy enabling label-free quantitative quality assessment one's model.

Table 4: **DIET is competitive and works out-of-the-box across architectures.** We keep the settings of Fig. 6, as per Table 1. Benchmarks from 1:[36], 2 :[37].

Imagenet-100 (IN100)								
Rest	iet18							
SimMoCo	58.20	-						
MocoV2	60.52	-	Resnet50					
SimCo	61.28	3*	MoCo+Hyper.	75.60 *				
W-MSE2	69.06	5^{2}	MoCo+DCL	76.80 *				
ReSSL	74.02	<u>2</u> •	MoCoV2 + Hy-	77.70 *				
DINO	74.16	5 •	per.					
MoCoV2	76.48	3∙	BYOL	$78.76^{\ 2}$				
BYOL	76.60		$M_0C_0V_2 + DCL$	80.50 *				
SimCLR	77.04	1^{2}	SimCLR	80.70 *				
SimCLR	78.72	2^{2}	SimSiam	81.60^{2}				
MocoV2	79.28	3^{2}	SimCLR + DCL	83.10 *				
VICReg	79.40	$)^{2}$	 					
BarlowTwins	80.38	3^{2}						
			ET					
resnet18		64.31	resnet50	73.50				
wide_resnet		71.92	convnext_small	71.06				
resnext50_32	2x4d	73.07	MLPMixer	56.46				
densenet121		67.46	swin_t	67.02				
convnext_tin	y	69.77	vit_b_16	62.63				

[103] (strength:3); the exact parameters for those transformations are given in Algorithm 3. We observe on TinyImagenet and with a Resnet34 the following performances 32.93 ± 0.6 , 45.60 ± 0.2 , and 45.75 ± 0.1 respectively over 5 independent runs, details and additional architectures provided in Fig. 9 and Table 3 in the Appendix. We thus observe that while DIET greatly benefit from richer DA (strength:1 \mapsto 2), it however does not require heavier transformation such as random erasing.

Label smoothing helps. One important difference in training behavior between supervised learning and SSL is in the number of epochs required to see the quality of the representation plateau. Due to the different loss used in DIET, one might wonder about the differences in training behavior. We observe that DIET takes more epochs than SSL until the loss converges. However, by using large values of label smoothing, *e.g.*, 0.8, it is possible to obtain faster convergence. We provide a sensitivity analysis in Fig. 8 and Table 3 in the Appendix. In fact, one should recall that within a single epoch, only one of each datum/class is observed, making the convergence speed of the classifier's W matrix the main limitation; we aim to explore improved training strategies in the future as discussed in Section 4.

Table 5: **DIET trained on small datasets competes with Imagenet pre-trained SSL.** We also report performances for a ViT based architecture (SwinTiny) to demonstrate the ability of DIET to handle different models out-of-the-box following Fig. 6. Benchmarks from \dagger :[34], +:[104]

Arch.	Pretrain	Frozen		<i>Aircraft</i> 6667 100			Flower 1020 102	CUB-200 11788 200	Food101 68175 101	Cars 6509 196
		Yes	SimCLR	24.19	54.35	46.46	75.00	16.73	-	-
Resnet18	IN100 [†]		+CLAE	25.87	52.12	43.55	76.82	17.58	-	-
Keshello			+IDAA	26.02	54.97	46.76	77.99	18.15	-	-
	None	No	DIET	37.29	50.62	64.06	72.01	33.03	62.00	42.55
			InsDis	36.87	68.46	68.78	83.44	-	63.39	28.98
			MoCo	35.55	68.83	69.84	82.10	-	62.10	27.99
			PCL.	21.61	62.87	75.34	64.73	-	48.02	12.93
			PIRL	37.08	68.99	71.36	83.60	-	64.65	28.72
			PCLv2	37.03	70.59	82.79	85.34	-	64.88	30.51
	DJ 11 +	1 + 37	SimCLR	44.90	74.20	83.33	90.87	-	67.47	43.73
	IN-1k ⁺	Yes	MoCov2	41.79	73.88	83.30	90.07	-	68.95	39.31
Resnet50			SimCLRv2	46.38	76.38	84.72	92.90	-	73.08	50.37
Resneiso			SeLav2	37.29	74.15	83.22	90.22	-	71.08	36.86
			InfoMin	38.58	74.73	86.24	87.18	-	69.53	41.01
			BYOL	53.87	76.91	89.10	94.50	-	73.01	56.40
			DeepClusterv2	54.49	78.62	89.36	94.72	-	77.94	58.60
			Swav	54.04	77.02	87.60	94.62	-	76.62	54.06
	None	No	DIET	44.81	51.75	67.08	73.32	41.03	71.58	55.82
SwinTiny	None	No	DIET	33.15	51.88	58.06	70.78	32.11	68.86	47.12
Convnext-S	None	No	DIET	43.13	49.52	61.72	67.72	31.44	69.84	40.63

E Linear Model Analysis

Let's consider the case of a linear model followed by the DIET loss. So the modeling loss given the data matrix $\boldsymbol{X} \in \mathbb{R}^{N \times D}$, the linear mapping matrix $\boldsymbol{V} \in \mathbb{R}^{D \times K}$ and the DIET linear probe matrix $\boldsymbol{W} \in \mathbb{R}^{N \times K}$, is of the form

$$\mathcal{L} = \text{CrossEntropy}(\boldsymbol{I}, \boldsymbol{X}\boldsymbol{V}\boldsymbol{W}^{\top})$$

= $\sum_{n=1}^{N} -(\boldsymbol{X}\boldsymbol{V}\boldsymbol{W}^{\top})_{n,n} + \log\left(\sum_{m=1}^{N} \exp((\boldsymbol{X}\boldsymbol{V}\boldsymbol{W}^{\top})_{n,m})\right)$
= $\sum_{n=1}^{N} -\langle(\boldsymbol{X}\boldsymbol{V})_{n,.}, (\boldsymbol{W})_{n,.}\rangle + \log\left(\sum_{m=1}^{N} \exp\left(\langle(\boldsymbol{X}\boldsymbol{V})_{n,.}, (\boldsymbol{W})_{m,.}\rangle\right)\right),$

the derivative with respect to the parameters V and W are given by

$$\nabla_{W} = AXV, \ \nabla_{V} = X^{\top}AW$$

where the matrix \boldsymbol{A} is given by

$$(\boldsymbol{A})_{i,j} = \left(\frac{e^{(\boldsymbol{X}\boldsymbol{V}\boldsymbol{W}^{\top})_{i,j}}}{\sum_{n=1}^{N} e^{(\boldsymbol{X}\boldsymbol{V}\boldsymbol{W}^{\top})_{i,n}}} - 1_{\{i=j\}}\right).$$

The above analysis is true for any matrix X, V, W. Finding a general solution by setting the gradient to 0 is not trivial due to the A matrix involving a softmax operation. However, for a special class of data matrices X, we are able to find a closed-form optimal solution for V and W. Let's now consider the following low-rank model for the input data matrix X as

$$\boldsymbol{X} \triangleq \left[\mu_1, \ldots, \mu_1, \ldots, \mu_K, \ldots, \mu_K\right]^+,$$

where each μ_i is repeated N/K times. That is, we assume that X has a low-rank structured made of "centroids". Note that while we assume here that each centroid is repeated the same number of times to simplify notations, none of the following results require uniform distribution of the centroids.

Then, DIET will effectively learn the clustering, as per the SVD of the data. In fact, let's consider the following parameters $V = V_X \Sigma_X^{-1}$ and $W = \kappa U_X$ where we used the (reduced) singular value

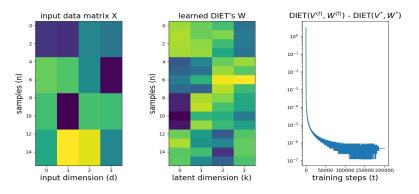
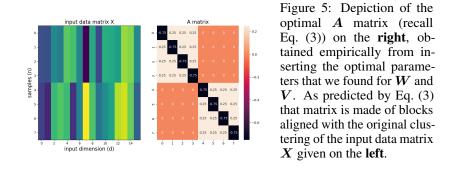


Figure 4: Empirical validation of Appendix E depicting the optimal solution for DIET for the parameters W and V under a clustered input data assumption (**left column**), in this case, made of four clusters with four samples per cluster. The learned W given in the **middle column** converge to the same clustering, as predicted by our closed-form solution. We also obtain in the **right column** the evolution of the DIET training loss that we compare against the optimal value of the loss (obtained from the optimal parameters). We see that the training converges towards the optimal value of the loss (up to 1e-7 at the end of that training episode).



decomposition of X as $X = U_X \Sigma_X V_X^{\top}$, and with $\kappa \gg 0$. In that setting, the matrix A becomes with a block structure as per

$$(\mathbf{A})_{i,j} = \frac{1}{K} \mathbb{1}_{\{[i/(N/K)] = [j/(N/K)]\}} - \mathbb{1}_{\{i=j\}},\tag{3}$$

as depicted in Fig. 5. This leads to a zero-gradient

$$\nabla_{\boldsymbol{W}} = \boldsymbol{0}, \nabla_{\boldsymbol{V}} = \boldsymbol{0}$$

effectively showing that we obtain the optimal parameters, as depicted in Fig. 4.

DIET's experimental setup:

- Official Torchvision architectures (no changes in init./arch.), only swapping the classification layer with DIET's one (right of Fig. 1), no projector DNN
- Same DA pipeline (\mathcal{T} in Fig. 1) across datasets/architectures with batch size of 256 to fit on 1 GPU
- AdamW optimizer with linear warmup (10 epochs) and cosine annealing learning rate schedule, XEnt loss (right of Fig. 1) with *label smoothing of* 0.8
- Learning rate/weight-decay of 0.001/0.05 for non transformer architectures and 0.0002/0.01 for transformers

Figure 6: In <u>underlined</u> are the design choices directly ported from standard supervised learning (not cross-validated for DIET), in *italic* are the design choices cross-validated for DIET but held constant across this study unless specified otherwise. Batch-size sensitivity analysis is reported in Table 3 and Fig. 9 showing that performances do not vary when taking values from 32 to 4096. XEnt's label smoothing parameter plays a role into DIET's convergence speed, and is cross-validated in Fig. 8 and Table 3; we also report DA ablation in Fig. 9 and Table 3.

F Code

Algorithm 2 Get the output dimension and remove the linear classifier from a given torchvision model (Pytorch used for illustration).

```
model = torchvision.models.__dict__[architecture]()
# CIFAR procedure to adjust to the lower image resolution if is_cifar and "resnet" in architecture:
    model.conv1 = torch.nn.Conv2d(3, 64, kernel_size=3, stride=1, padding=2, bias=False)
    model.maxpool = torch.nn.ldentity()
\# for each architecture, remove the classifier and get the output dim. (K)
if "alexnet" in architecture
    K = model.classifier[6].in_features
    model.classifier[6] = torch.nn.ldentity()
      "convnext" in architecture:
elif
    K = model. classifier [2]. in_features
    model.classifier [2] = torch.nn.ldentity()
elif "convnext" in architecture:
    K = model. classifier [2].in_features
    model.classifier [2] = torch.nn.ldentity()
   K = model.fc.in_features
elif
    model.fc = torch.nn.ldentity()
"densenet" in architecture:
elif
    K = model. classifier.in_features
    model.classifier = torch.nn.ldentity()
   mobile" in architecture:
K = model.classifier[-1].in_features
elif
model.classifier[-1] = torch.nn.ldentity()
elif "vit" in architecture:
    \mathsf{K} = \mathsf{model.heads.head.in\_features}
    model.heads.head = torch.nn.ldentity()
۵lif
      "swin" in architecture:
    \mathsf{K} = \mathsf{model.head.in\_features}
    model.head = torch.nn.ldentity()
```

F.1 Pushing the DIET to Large Models and Datasets

Given DIET's formulation of considering each datum as its own class, it is natural to ask ourselves how scalable is such a method. Although we saw that on small and medium scale dataset, DIET's was able to come on-par with most current SSL methods, it is not clear if this remains true for larger datasets. In this section we briefly describe what can be done to employ DIET on datasets such as Imagenet and INaturalist.

The first dataset we consider is INaturalist which contains slightly more than 500K training samples for its mini version (the one commonly employed, see *e.g.* [14]). It contains almost 10K actual classes and most SSL methods focus on transfer learning *e.g.* transferring with a Resnet50 from Imagenet-1k lead to SimCLR's 37.2%, MoCoV2's 38.6, BYOL's 47.6 and BarlowTwins'46.5. However training on INaturalist directly produces lower performances reaching only 29.1 with MSN and a ViT. Using DIET is possible out-of-the-box with Resnet18 and ViT variants as their embedding is of dimension

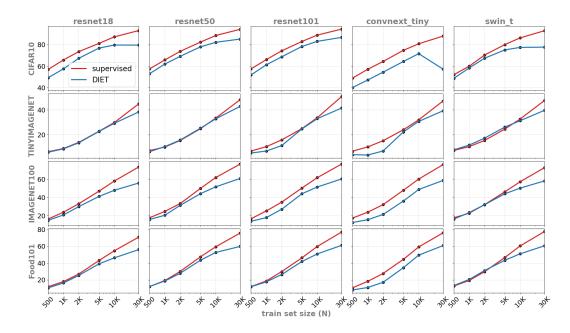


Figure 7: Reprise of Appendix D on additional datasets depicting how DIET is able to compete with supervised learning for in-distribution generalization in very small dataset regime.

512 and 762 respectively making W fit in memory. We obtain 22.81 with a convnext small, and 21.6 with a ViT.

The second dataset we consider is the full Imagenet-1k dataset which contains more than 1 million training samples and 1000 actual classes. In this case, it is not possible to directly hold W in-memory. We however tried a simple strategy which simply consists of sub-sampling the training set to a more reasonable size. This means that although we are putting aside many training images, we enable single GPU Imagenet training with DIET. With a training size of 400K, we able to reach 44.05 with a convnext small, 43.78 with a SwinTiny, and 44.89 with a ViT/B/16. A standard SSL pipeline has performances ranging between 64% and 72%. From those experiments, it is clear that DIET's main limitation comes from very large training set sizes. Although the above simple strategy offers a workable solution, it is clearly not sufficient to match with existing unsupervised learning method and thus should require further consideration. As highlighted in Section 4 below, this is one key avenue for future work.

G Impact of Training Time and Label Smoothing

In Figure 8 we show the performance of DIET on CIFAR100 across three label smoothing settings. We find higher values of label smoothing speed up convergence, although in this setting all cases greatly benefit from longer training schedules; final linear probe performances are reported in Table 3.

H Impact of Mini-Batch Size

We show in 9 ablations for TinyImagenet using DIET. In addition we show DIET"s robustness to batch size by conducting an additional ablation by varying the batch size for the Derma MedMNIST dataset with batch sizes as low as 8. As shown in Table 6, we see DIET performs well even with very small batch sizes.

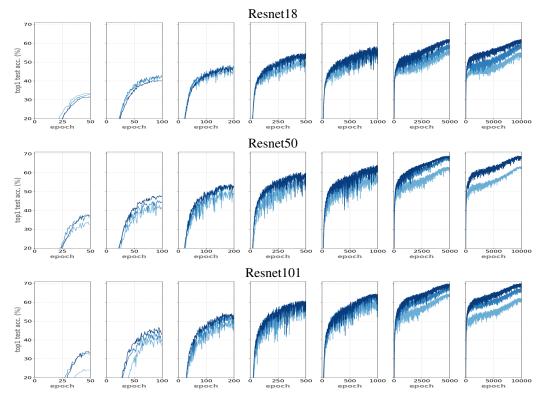


Figure 8: Depiction of the evolution of linear top1 accuracy throughout epochs on CIFAR100 with three Resnet variants and three label smoothing parameters represented by the different **shades of blue** going from light to dark shades with values of 0.1, 0.4, and 0.8 respectively.

Batch Size	8	32	64	128	512
DIET	71.87	72.52	73.07	74.36	71.02
MoCov2	66.88	64.64	66.73	66.88	61.40
SimCLR	63.14	66.43	66.83	66.88	66.83
VICReg	65.84	60.45	64.79	66.78	66.88

Table 6: Reprise of Table $\overline{3: \text{ DIET's performance across varying batch sizes on the Derma MedMNIST dataset with all other hyperparameter fixed demonstrating the stability of DIET do that hyperparameter and across training iterations. All models are trained for 500 epochs.$

I Impact of Data-Augmentation

To further study the effect of data augmentation in DIET we study varying data augmentation strengths for TinyImageNet in Fig. 9. We also examine the effect of weaker data augmentations for smaller medical images using PathMNIST in Table 7.

J DIET compared to supervised learning

DIET matches supervised learning on datasets with only a few samples per class. In Appendix D we directly compare DIET with supervised learning on a variety of models and datasets but with controlled training size. We clearly observe that for small dataset, *i.e.*, for which we only use a small part of the original training set (less than 30 images per class), DIET's learned representation is as efficient as the supervised one for the in-distribution classification downstream task.

DIET works with scattering network architectures As an additional test, scattering networks [105, 106] hard-code part of the model parameters to be wavelet filter-banks. That specification naturally makes such scattering networks very competitive for small data regimes since the number of

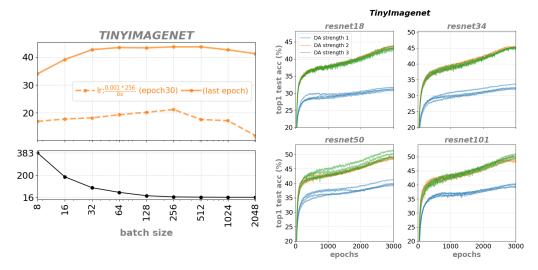


Figure 9: Left:TinyImagenet with fixed number of epochs and a single learning rate which is adjusted for each case using the LARS rule therefore per batch-size learning cross-validation can only improve performances, see Table 3, the per-epoch time includes training, testing, and checkpointing. **Right:** TinyImagenet, see Table 3 for table of results, and the specific DAs can be found in Algorithm 3.

Algorithm 3 Custom dataset to obtain the indices (n) in addition to inputs x_n and (optionally) the labels y_n to obtain train_loader used in ?? (Pytorch used for illustration).

```
transforms = [
    RandomResizedCropRGBImageDecoder((size, size)),
    RandomHorizontalFlip(),
]
if strength > 1:
    transforms.append(
        T.RandomApply(
            torch.nn.ModuleList([T.ColorJitter(0.4, 0.4, 0.4, 0.2)]), p=0.3
    )
    )
    transforms.append(T.RandomGrayscale(0.2))
if strength > 2:
    transforms.append(
        T.RandomApply(
            torch.nn.ModuleList([T.GaussianBlur((3, 3), (1.0, 2.0))]), p=0.2
    )
    )
    transforms.append(T.RandomErasing(0.25))
```

degrees of freedom is reduced. We therefore performed two additional experiments: Training a hybrid scattering network in a supervised setting Training a hybrid scattering network with DIET and then learning a linear probe on top (keeping the hybrid scattering frozen) We perform both cases above on the full CIFAR10 training set and on a reduced training set of 5000 (10% of the training data) samples. Supervised training of the scattering network results in 72.1% (58.2%) test set accuracy, whereas unsupervised DIET pretraining followed by a linear probe results in 77.64% (62.8%) for the same architecture. From that experiment we obtain two novel insights. First, DIET works out-of-the-box on DNs such as the hybrid scattering network, with a reduced number of parameters. Second, even in that regime, DIET provides strong performances.

K Additional Results for MedMNIST

In Figure 10 we show training curves for DIET with a ResNet18 architecture. We perform additional experiments with DIET using a vision transformer architecture (ViT-Small with patch size 4) based on the architecture from https://github.com/lucidrains/vit-pytorch/blob/main/vit_pytorch/vit_for_small_dataset.py. We find DIET achieves good performance on the same MedMNIST datasets with this ViT architecture without additional hyperparameter tuning as shown in Table 8 and in comparison to all three baseline SSL methods in Table 7.

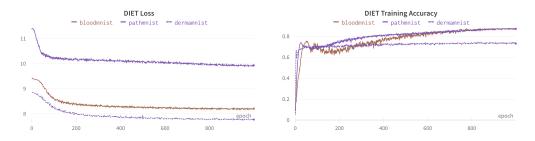


Figure 10: DIET MedMNIST training loss curves for the DIET criterion (left) and training accuracy (right) with a ResNet18 backbone.

	bloodmnist		derma	nmnist	pathmnist		
	train	test	train	test	train	test	
DIET	77.65	81.85	71.03	68.88	56.37	21.27	
SimCLR	82.48	79.45	69.13	32.37	69.45	21.80	
VICReg	86.71	81.03	69.89	46.33	82.94	12.76	
MoCov2	62.76	51.01	66.78	63.39	72.9	41.75	
	DIET		PathMNIST		-		
	Augme	entation	train	test	-		
	Default		56.37	21.27			
	Weak		44.90	48.95			
	None		44.65	45.67			

Table 7: **Top:**DIET performance across the three MedMNIST datasets using a transformer (ViT-S) architecture with patch size 4 in comparison to standard SSL baselines with the same ViT architecture. **Bottom:**Comparing DIET's performance across data augmentations for PathMNIST using a transformer (ViT-S) architecture with patch size 4. Weak augmentation corresponds to only random resized cropping and horizontal flipping.

Table 8: DIET performance across the three MedMNIST datasets using a transformer (ViT-S) architecture with patch size 4. In the first row we show the performance of a baseline SimCLR model with the default ResNet18 encoder for comparison.

dataset					pathmnist		
	train	test	train	test	train	test	
DIET	77.65	81.85	71.03	68.88	56.37	21.27	

We find evidence of the default augmentations for PathMNIST being too aggressive and confirm DIET's performance improves with the use of weaker augmentations in Table 7. Surprisingly, we find DIET performs quite well with no augmentations at all, a setting in which most standard SSL methods would be impossible to train.

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