Predicting is not Understanding: Recognizing and Addressing Underspecification in Machine Learning

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Abstract. Machine learning (ML) models are typically optimized for their accuracy on a given dataset. However, this predictive criterion rarely captures all desirable properties of a model, in particular how well it matches a domain expert's *understanding* of a task. Underspecification [6] refers to the existence of multiple models that are indistinguishable in their in-domain accuracy, even though they differ in other desirable properties such as out-of-distribution (OOD) performance. Identifying these situations is critical for assessing the reliability of ML models. We formalize the concept of underspecification and propose a method to identify and partially address it. We train multiple models with an independence constraint that forces them to implement different functions. They discover predictive features that are otherwise ignored by standard empirical risk minimization (ERM), which we then distill into a global model with superior OOD performance. Importantly, we constrain the models to align with the data manifold to ensure that they discover meaningful features. We demonstrate the method on multiple datasets in computer vision (collages, WILDS-Camelyon17, GQA) and discuss general implications of underspecification. Most notably, in-domain performance cannot serve for OOD model selection without additional assumptions.[1]

1 Introduction

Is data all you need? A finite set of i.i.d. examples is almost never sufficient to learn a task. Inductive biases have long been known to be necessary for in-domain generalization [32,54]. OOD[2] generalization complicates things further since one also needs to determine which predictive patterns of the training data will remain relevant at test time. Correlations between inputs and labels that are important for the task may be indistinguishable from spurious ones that result from dataset-specific artefacts such as selection biases.

An example in image recognition. Image labels are often correlated with objects and the backgrounds they appear in (*e.g.* cars in cities, birds in nature). Recognizing either often suffice to predict correct labels. However, robust OOD

[1]See https://arxiv.org/abs/2207.02598 for the full-length version of this work.
[2]In this paper, OOD means there is a covariate shift between training and test data [44].

generalization (*e.g.* correctly labeling images of birds in street scenes) requires to rely on shapes and to ignore the background. When this requirement cannot be deduced from the data (because both features leave a similar signature in the joint training distribution), the task is said to be underspecified. In this example, the task requires the additional knowledge that labels refer to object shapes rather than background textures [12]. Such knowledge is often task-specific. For example, the opposite choice of prioritizing color or texture over shape would be sensible for recognizing traffic signs or segmenting medical images.

Underspecification gap: the difference between the information provided in a dataset and the information required to perform *as desired* on a task.

The qualifier "*as desired*" captures the fact that different use cases require different properties such as adversarial robustness, interpretability, fairness, or OOD generalization. The latter is the focus of this paper. Underspecification arises because these properties do not necessarily correlate with the ERM objective [50] typically used to train models.

This paper argues that **identifying underspecification** is important for assessing the reliability of ML models, their reliance on hidden assumptions, and for identifying the information missing for OOD robustness. We identify underspecification by **discovering multiple understandings** of the data. We learn multiple predictive models compatible with a given dataset and hypothesis class (low in-domain risk). We force them to rely on different predictive features by encouraging orthogonality of their input gradients. We also ensure that these features remain semantically meaningful by constraining the input gradients to the data manifold. Training multiple models stands in contrast with the standard practice of optimizing a single solution to a learning problem – which hides the existence of underspecification. With our method, we discover predictive features otherwise ignored by standard ERM. This alone produces candidate models with superior OOD performance. In addition, we show how to distill selected features from multiple candidate models into one that is robust across a wider range of distribution shifts. In all cases, a selection strategy must be provided such as an OOD validation set, domain expertise, task-specific heuristics, etc.

Experiments. We apply the method to controlled data (collages [43,48]) and computer vision benchmarks (WILDS-Camelyon17 [27], GQA [20,24]). On visual question answering, we show that multiple models can produce similar answers while relying on different visual features (Figure 1).

Implications. Our work complements other studies [6,30] in formalizing underspecification as a root cause of multiple challenges in ML including shortcut learning, distribution shifts, and even adversarial vulnerabilities (an extreme case of OOD inputs). Our formalization of underspecification makes it obvious that ID and OOD performance are not necessarily coupled. Therefore, without further assumptions, in-domain validation performance is not a reliable model selection strategy for OOD performance despite contradictory suggestions made in the literature [16,31]. The prevalence of underspecification [6] also suggests that

Fig. 1: Example of underspecification in visual question answering. Our method trains multiple models that each discover different predictive features. We obtain three models producing identical answers on most training and validation data, even though they rely on different visual clues (evidenced by grad-CAM visualizations over object proposals [41]). Each model reflects a **different understanding of the task** compatible with the data (possibly incomprehensible to humans) which reveals ambiguity in its specification.

task-specific knowledge and assumptions are often necessary to build robust ML models, since they cannot emerge from simply scaling up data and architectures. We summarize our contributions as follows. See the supp. mat. for related work.

1. We propose a mathematical framework for quantifying and addressing underspecification.
2. We derive a method to learn a set of models compatible with a given dataset that exhibit distinct OOD behaviour. We force the models to rely on different features (independence objective) that are nonetheless semantically meaningful (on-manifold constraint).
3. We use the method for (1) highlighting underspecification in given dataset/architecture pairs, and (2) building models with superior OOD performance on collages [43,48], WILDS-Camelyon17 [27], and GQA [20,24].

2 Formalizing underspecification

Let us focus on binary classification tasks. A dataset provides **labeled examples** $\mathcal{D}_{\text{tr}} = \{(\boldsymbol{x}_i, y_i)\}_i$ with $\boldsymbol{x} \in \mathbb{R}^{d_{\text{in}}}$, $y_i \in \{0,1\}$. The goal of a learning algorithm is to identify a **predictor** $f : \mathbb{R}^{d_{\text{in}}} \to \mathbb{R}$ to estimate labels[3] of examples from a test set $\mathcal{D}_{\text{test}} = \{\boldsymbol{x}_i\}_i$. While the input data $\boldsymbol{x}$ is typically high-dimensional (*e.g.* vectorized images), natural data (*e.g.* photographs) occupies only a fraction of the input space assumed to form a low-dimensional **manifold** [53] $\mathcal{M} \subset \mathbb{R}^{d_{\text{in}}}$. The dimensionality d_{manifold} ($< d_{\text{in}}$) is known as the **intrinsic dimensionality** of the data. Training and test data are drawn from a distribution on this manifold P_{ID} (in-domain examples) while unbiased natural data (free of dataset-specific selection biases) is drawn from a distribution P_{OOD} of typically broader support.

[3] We define f to output logits. A binary prediction $\hat{y}$ is obtained as $\hat{y} = \text{round}\left(\sigma\left(f(\boldsymbol{x})\right)\right)$.

Inductive biases are the properties of a learning algorithm that determine what model $f_{\theta^\star}$ is returned for a dataset $\mathcal{D}$ from a hypothesis class $\mathcal{H} = \{f_{\boldsymbol{\theta}}, \forall\, \boldsymbol{\theta}\}$ where $f_{\boldsymbol{\theta}}$ is a model with free parameters θ. Inductive biases enable generalization from finite data [32] by encoding assumptions on the relation between $\mathcal{D}$ and $\mathcal{D}_{\text{test}}$. In particular, classical learning theory assumes that $\mathcal{D}$ and $\mathcal{D}_{\text{test}}$ contain i.i.d. samples from the same distribution. For completeness, we summarize a standard training workflow.

1. Randomly split the data into training and validation sets: $\mathcal{D} = \mathcal{D}_{\text{tr}} \cup \mathcal{D}_{\text{val}}$.
2. A **hypothesis class** $\mathcal{H} = \{f_{\boldsymbol{\theta}}, \forall\, \boldsymbol{\theta}\}$ is chosen *e.g.* by defining a neural architecture f.
3. **Empirical risk minimization** serves to optimize the free parameters of f as $\boldsymbol{\theta}^\star = \text{argmin}_{\boldsymbol{\theta}}\ \mathcal{R}\left(f_{\boldsymbol{\theta}}, \mathcal{D}_{\text{tr}}\right)$ where the empirical risk is defined as $\mathcal{R}(f, \mathcal{D}) = \Sigma_{(\boldsymbol{x},y)\in\mathcal{D}}\ \mathcal{L}_{\text{pred}}\big(y, \sigma\big(f(\boldsymbol{x})\big)\big)\ /\ |\mathcal{D}|$,
and $\mathcal{L}_{\text{pred}}$ is a predictive loss such as binary cross-entropy.
4. **Validation performance** serves to refine various choices (architecture, regularizers, …) by trial and error, *i.e.* loosely solving $f'_{\boldsymbol{\theta}^{\star\prime}} = \text{argmin}_{f,\ldots}\, \mathcal{R}(f_{\boldsymbol{\theta}^\star}, \mathcal{D}_{\text{val}})$ where $\mathcal{R}$ is often substituted with a task-specific metric such as the error rate.

There is often a multitude of models satisfying the above procedure, not all are equally desirable because they differ in properties that the procedure does not constrain. The degree of underspecification indicates the importance of arbitrary and stochastic factors in the outcome of the learning process.

This paper focuses on **differences in OOD performance** among predictive models. OOD performance is the predictive performance of a model (in terms of risk, accuracy, or another task-specific metric) on test data drawn from a distribution $\text{P}_{\text{OOD}} \neq \text{P}_{\text{ID}}$. On OOD data, features that were predictive in the training data may become irrelevant or misleading, causing a drop in performance of a model that relies on them. By definition, OOD performance is underspecified by the ERM objective, since the empirical risk is estimated on in-domain data.

To capture variability in OOD performance, we propose a definition of underspecification based on the number of ways to fit the data with the above procedure and produce different OOD predictions.[4]

Definition 1. *The* ***degree of underspecification*** *of a dataset* $\mathcal{D} = \mathcal{D}_{\text{tr}} \cup \mathcal{D}_{\text{val}}$*, input manifold* $\mathcal{M}$*, and hypothesis class* $\mathcal{H} = \{f_{\boldsymbol{\theta}}, \forall\, \boldsymbol{\theta}\}$ *is the ratio of volumes* $vol(\mathcal{H}')/\, vol(\mathcal{H})$ *of the largest subset of models* $\mathcal{H}' \subset \mathcal{H}$ *such that its elements* $\{f_{\boldsymbol{\theta}_m}\}_m$ *all have, for small constants* ϵ_{tr}, ϵ_{val}*:*

- *A low training risk:* $\mathcal{R}(f_{\boldsymbol{\theta}_m}, \mathcal{D}_{\text{tr}}) < \epsilon_{tr},\ \forall\, f_{\boldsymbol{\theta}} \in \mathcal{H}'$,
- *A low validation risk:* $\mathcal{R}(f_{\boldsymbol{\theta}_m}, \mathcal{D}_{\text{val}}) < \epsilon_{val},\ \forall\, f_{\boldsymbol{\theta}} \in \mathcal{H}'$,
- *Distinct OOD predictions:* $P\big(\text{round}(\sigma(f_{\boldsymbol{\theta}1}(\boldsymbol{x})) \neq \text{round}(\sigma(f_{\boldsymbol{\theta}2}(\boldsymbol{x}))\big) \approx 1$, $\forall\ f_{\boldsymbol{\theta}1}, f_{\boldsymbol{\theta}2} \in \mathcal{H}',\quad f_{\boldsymbol{\theta}1} \neq f_{\boldsymbol{\theta}2},\quad \boldsymbol{x} \sim P_{\text{OOD}}$.

The next section derives a method to learn a set of models with these properties.

[4] Previously, [19,42] used volumes of hypothesis spaces to define Rashomon sets.

3 Proposed method

Overview. We train multiple models with the same architecture and data while enforcing them to represent different functions and use different features. The models use different initializations, but this does not always suffice to produce significantly-different models. We add two regularizers that enforce (1) independence of the models (mutually-orthogonal input gradients) and (2) alignment with the data manifold such that the models learn meaningful features.

Since the constraints follow from Definition 1, the number of models trainable to satisfy them indicates the degree of underspecification. The only existence of multiple such models thus highlights cases of underspecification. The models also discover some predictive features missed by standard ERM, which can be combined by distillation into a predictor with superior OOD performance. In the next sections, we implement the two constraints as differentiable regularizers.

3.1 Independent models

To optimize for distinct OOD predictions, we turn the criteria of Definition 1 into a differentiable objective using the concept of independent models [39,40].

Definition 2. *A pair of predictors $f_{\boldsymbol{\theta}_1}$, $f_{\boldsymbol{\theta}_2}$ are **locally independent** at $\boldsymbol{x}$ iff their predictions are statistically independent for Gaussian perturbations around $\boldsymbol{x}$: $f_{\boldsymbol{\theta}_1}(\widetilde{\boldsymbol{x}}) \perp f_{\boldsymbol{\theta}_2}(\widetilde{\boldsymbol{x}})$, $\widetilde{\boldsymbol{x}} \sim \mathcal{N}(\boldsymbol{x}, \sigma \boldsymbol{I})$.*

Definition 3. *A set of predictors $\{f_{\boldsymbol{\theta}_1}, ..., f_{\boldsymbol{\theta}_M}\}$ are **globally independent** on a dataset $\mathcal{D}$ iff every pair of them are locally independent at every $\boldsymbol{x} \in \mathcal{D}$.*

This formalizes the notion that models can rely on different features. In our case, we seek a set of models globally independent from one another. We obtain a tractable objective using the relation between statistical independence and geometric orthogonality developed in [40].

Proposition 1. *A pair of predictors $f_{\boldsymbol{\theta}_1}$, $f_{\boldsymbol{\theta}_2}$ are locally independent at $\boldsymbol{x}$ iff the mutual information $MI(f_{\boldsymbol{\theta}_1}(\widetilde{\boldsymbol{x}}), f_{\boldsymbol{\theta}_2}(\widetilde{\boldsymbol{x}})) = 0$ with $\widetilde{\boldsymbol{x}} \sim \mathcal{N}(\boldsymbol{x}, \sigma \boldsymbol{I})$.*

For infinitesimally small perturbations ($\sigma \to 0$), samples $\widetilde{\boldsymbol{x}}$ can be approximated through linearization by the input gradients $\nabla_{\boldsymbol{x}} f$. These are 1D Gaussian random variables whose correlation is given by $\cos\left(\nabla_{\boldsymbol{x}} f_{\boldsymbol{\theta}_1}(x), \nabla_{\boldsymbol{x}} f_{\boldsymbol{\theta}_2} x\right)$. Their mutual information [15] is $-\frac{1}{2}\ln\left(1 - \cos^2\left(\nabla_{\boldsymbol{x}} f_{\boldsymbol{\theta}_1}(x), \nabla_{\boldsymbol{x}} f_{\boldsymbol{\theta}_2}(x)\right)\right)$. Therefore, the statistical independence between the models' outputs as their inputs are perturbed by small Gaussian variations can be enforced by making their input gradients orthogonal. Our **local independence loss** for a pair of models is:

$$\mathcal{L}_{\text{indep}}\left(\nabla_{\boldsymbol{x}} f_{\boldsymbol{\theta}_{m_1}}(\boldsymbol{x}),\ \nabla_{\boldsymbol{x}} f_{\boldsymbol{\theta}_{m_2}}(\boldsymbol{x})\right) \;=\; \cos^2\left(\nabla_{\boldsymbol{x}} f_{\boldsymbol{\theta}_{m_1}}(\boldsymbol{x}),\ \nabla_{\boldsymbol{x}} f_{\boldsymbol{\theta}_{m_2}}(\boldsymbol{x})\right) \tag{1}$$

with $\cos^2(\boldsymbol{v}, \boldsymbol{w}) = (\boldsymbol{v}^\intercal \boldsymbol{w})^2 \,/\, (\boldsymbol{v}^\intercal \boldsymbol{v})(\boldsymbol{w}^\intercal \boldsymbol{w})$. To enforce *global* independence, this loss will be applied to all training points and pairs of models in Eq. (3).

3.2 On-manifold constraint

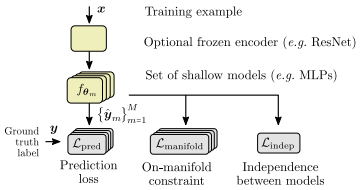


Fig. 2: Method overview during training.

The independence constraint (1) makes models' input gradients orthogonal to one another. The number of models satisfying it grows exponentially with the input dimension (d_{in}) but many are practically irrelevant because the natural data manifold usually occupies much fewer dimensions. Intuitively, when the constraint affects a model's gradients in dimensions pointing outward the manifold, it does not affect its predictions on natural data. Consequently, the independence constraint could be satisfied by models that produce identical predictions on every natural input (thus defeating its purpose) because their decision boundaries are identical when projected on the manifold. The issue stems from the *isotropic* perturbations in Eq. (1). Only perturbations *on* the manifold are meaningful.

One straightforward solution would be to enforce independence after projecting the data on a learned approximation of the manifold. This approach, proposed in [39,40] failed in our early experiments because of the difficulty of optimizing the independence objective under such a strict on-manifold constraint. Instead, we implement a soft constraint as a regularizer that proved easy to train and resilient to imperfect models of the manifold.

To learn the data manifold $\mathcal{M}$, we need unlabeled examples, ideally containing the type of OOD data expected at test time *e.g.* a broad collection of natural images: $\mathcal{D}_{\text{OOD}} = \{\boldsymbol{x}_i\} \sim \text{P}_{\text{OOD}}$. We use this data off-line to prepare a function $\text{proj}_{\mathcal{M}}(\boldsymbol{x}, \boldsymbol{v})$ that projects an arbitrary vector $\boldsymbol{v}$ at $\boldsymbol{x}$ in the input space onto the manifold (Figure 3). During training, we penalize each model with the distance between its input gradients and their projection on the manifold. The **on-manifold loss** is defined as

$$\mathcal{L}_{\text{manifold}}\big(\nabla f(\boldsymbol{x})\big) = \Big|\Big|\text{proj}_{\mathcal{M}}\big(\boldsymbol{x}, \nabla_{\boldsymbol{x}} f(\boldsymbol{x})\big) - \nabla_{\boldsymbol{x}} f(\boldsymbol{x})\Big|\Big|_2^2. \tag{2}$$

We describe possible implementations of $\text{proj}_{\mathcal{M}}(\cdot)$ in the supp. mat. with a variational auto-encoder (VAE) or a simple PCA. In summary, the on-manifold loss encourages a model to be sensitive to variations in the input that are likely to be encountered in natural test data. It typically has no effect on in-domain performance (Figure 6c) since it only removes a model's sensitivity to unnatural inputs such as variations of isolated pixels unlikely to appear in natural images.

The overall learning objective combines the predictive, independence, and on-manifold losses:

$$\begin{aligned}\mathcal{L}(\mathcal{D}_{\text{tr}}, \boldsymbol{\theta}_1 \dots \boldsymbol{\theta}_M) = \Sigma_{\boldsymbol{x} \in \mathcal{D}_{\text{tr}}} \Big[\quad & (1/M) \quad \Sigma_{m=1}^{M} \mathcal{L}_{\text{pred}}\big(y,\, \sigma(f_{\boldsymbol{\theta}_m}(\boldsymbol{x}))\big) \\ & + (1/M^2) \; \Sigma_{m_1=1}^{M} \Sigma_{m_2=1}^{M} \lambda_{\text{indep}} \;\; \mathcal{L}_{\text{indep}}\big(\nabla_{\boldsymbol{x}} f_{\boldsymbol{\theta}_{m_1}}(\boldsymbol{x}), \nabla_{\boldsymbol{x}} f_{\boldsymbol{\theta}_{m_2}}(\boldsymbol{x})\big) \\ & + (1/M) \quad \Sigma_{m=1}^{M} \lambda_{\text{manifold}} \;\; \mathcal{L}_{\text{manifold}}\big(\nabla_{\boldsymbol{x}} f_{\boldsymbol{\theta}_m}(\boldsymbol{x})\big) \; \Big].\end{aligned} \tag{3}$$

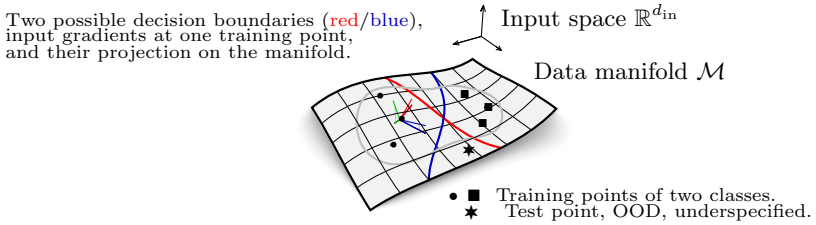


Fig. 3: Effect of the proposed method in input space. Data such as natural images is assumed to lie on a low-dimensional manifold. The training set covers a subset of this manifold (gray ellipse). OOD test data (★) lies outside this subset. In this example, our method discovers two models (red and blue decision boundaries) whose input gradients are orthogonal (shown at one training point, in colors matching the boundary). Even though a third model (green vector) could satisfy the orthogonality constraint, its input gradient would point outside the manifold. This would violate the *on-manifold* constraint, which requires gradients to closely match their projection on the manifold.

3.3 Fine-tuning

After training a set of models with (3), we propose to relax the independence and on-manifold constraints ($\lambda_{\text{indep}} \leftarrow 0$, $\lambda_{\text{manifold}} \leftarrow 0$) then fine-tune the models. This eases the optimization and typically allows the models to reach a higher predictive accuracy. Concretely, we apply binary masks on the data such that each model is fine-tuned only on the elements most relevant to itself:[5]

$$\mathcal{D}_{\text{tr}}^m = \{(\boldsymbol{x}_i \odot \mathbf{mask}_i^m, y_i) : (\boldsymbol{x}_i, y_i) \in \mathcal{D}_{\text{tr}}\} \tag{4}$$

with $\mathbf{mask}_i^m \in \{0,1\}^{d_{\text{in}}}$. They are computed before starting the fine-tuning to highlight the data most relevant to each model. Each element (pixel, channel) is unmasked only for the model with the largest corresponding gradient magnitude:

$$\mathbf{mask}_i^m = \mathbb{1}\big(m = \underset{1 \leqslant m \leqslant M}{\operatorname{argmax}} \nabla f_{\boldsymbol{\theta}_m}(\boldsymbol{x}_i)\big) \quad \forall\, (\boldsymbol{x}_i, \cdot) \in \mathcal{D}_{\text{tr}}. \tag{5}$$

We fine-tune each model on its own masked version of the data.[6] This ensures that the models remain distinct despite disabling the regularizers ($\lambda_{\text{indep}} \leftarrow 0$, $\lambda_{\text{manifold}} \leftarrow 0$). See Algorithm 1 for a summary.

3.4 Distilling multiple models into one

Finally, after training/fine-tuning a set of models, we propose to combine the best of them into a global one that uses all of the most relevant features.We train this global model from scratch, without regularizers, on masked data as described above, using masks from *multiple* selected models combined with a

[5] In our implementation, masked elements are not replaced with zeros, but rater with random values from other instances in the current mini-batch.

[6] We obtain very similar results between fine-tuning and retraining models from scratch on the masked data.

Algorithm 1: Training and fine-tuning models.

Inputs: Labeled examples $\mathcal{D}_{\text{tr}}$. Unlabeled examples $\mathcal{D}_{\text{OOD}}$ (typically $\mathcal{D}_{\text{tr}} \subset \mathcal{D}_{\text{OOD}}$). Architecture f.
Result: Set of independent models $\{f_{\boldsymbol{\theta}_1} \dots f_{\boldsymbol{\theta}_M}\}$.
Method:
With $\mathcal{D}_{\text{OOD}}$, estimate dimensionality d_{manifold} [37] and set the number of models $M \leftarrow d_{\text{manifold}}$.
With $\mathcal{D}_{\text{OOD}}$, prepare function proj$(\cdot)$ by PCA decomp. or by training a VAE.
With $\mathcal{D}_{\text{tr}}$, train M instances of f in parallel (Eq. 3):
$\{\boldsymbol{\theta}_1 \dots \boldsymbol{\theta}_M\} \leftarrow \text{argmin}\, \mathcal{L}(\mathcal{D}_{\text{tr}}, \boldsymbol{\theta}_1 \dots \boldsymbol{\theta}_M)$.
Determine masks on input data (Eq. 5): $\{\mathbf{mask}_i^m\}_{i,m}$
foreach m **do** // Optional fine-tuning on masked data
  $\mathcal{D}_{\text{tr}}^m \leftarrow \{(\boldsymbol{x}_i \odot \mathbf{mask}_i^m, y_i)\}_i$ // Prepare masked data
  $\lambda_{\text{indep}} \leftarrow 0,\ \lambda_{\text{manifold}} \leftarrow 0$ // Use only predictive loss
  $\boldsymbol{\theta}_m \leftarrow \text{argmin}\, \mathcal{L}(\mathcal{D}_{\text{tr}}^m, \boldsymbol{\theta}_m)$ // Fine-tune

logical OR. In our experiments, we combine the two models with the highest accuracies on an OOD validation set. We repeat this pairwise combination as long the accuracy of the global model increases, usually for 2–3 iterations (as formalized in the supp. mat.).

4 Experiments

We first present experiments that validate the method on controlled data with multiple known features (collages, Section 4.1). We then demonstrate applications to existing datasets: WILDS-Camelyon17 (Section 4.2) and GQA (see the supp. mat.).

4.1 Experiments on controlled data: collages

This diagnostic dataset contains images with binary labels that are constructed to contain multiple predictive features [43,48]. Each image contains four tiles representing one of two classes respectively from MNIST (0/1), CIFAR-10 (automobile/truck), Fashion-MNIST (pullover/coat), and SVHN (0/1).

- At **training time**, the labels are perfectly correlated with the four tiles (0/1 respectively for the first/second possible class in each tile). There are (at least) four equally-valid ways of understanding the task (*i.e.* relying on any of the four tiles).
- At **test time**, we evaluate a model on four test sets that represent different OOD conditions. In each, only one tile is correlated with the correct label while others tiles are randomized. By examining the performance on the four test sets, we can identify which tile(s) the model relies on

Task difficulty. This dataset is surprisingly challenging because the tiles vary greatly in learning difficulty (*e.g.* MNIST 0s/1s are very distinct while

Fig. 4: Examples of collages [48]. Tr. labels are correlated with all four tiles.

Fashion-MNIST pullovers/coats look extremely similar). It would be reasonable to learn a model that relies on all four tiles. However, an ERM-trained baseline surprisingly uses only a few MNIST pixels (achieving ∼99% accuracy on the MNIST test set and ∼50% on the others), as shown in previous work on the simplicity bias of neural networks [48].

We follow [48] and use our method to learn multiple models compatible with the data. We then report the accuracy of the best model on each test set, *i.e.* the best accuracy assuming perfect model selection. This avoids confounding the performance of the learning algorithm and with that of the selection strategy.

Applying the proposed method. We follow Algorithm 1. We prepare unlabeled data to defines the data manifold as the union of the training and test sets, thus covering all combinations of contents of the four tiles. With this data, we estimate the dimensionality of the manifold with [37] as about 23.8 ($\sigma = 0.16$ over 10 runs). We prepare two generative models of the manifold: a PCA with 24 components (capturing ∼85% of the variance) and a VAE with 24 latent dimensions (details in the supp. mat.). We define a simple architecture (2-layer MLPs) and train multiple instances in parallel with the proposed objective. The only hyperparameters are the number of models and weights of independence/on-manifold constraints. We plot a range of values in the supp. mat.

Results. Our method learns models that focus on different parts of the images. Remarkably, learning as few as 4 models is sufficient to obtain models with high accuracy on all of four test sets. Let us examine several ablations.

- The baseline ($\lambda_{\text{indep}} = \lambda_{\text{manifold}} = 0$) only learns about MNIST.
- The independence constraint ($\lambda_{\text{indep}} >$, $\lambda_{\text{manifold}} = 0$) is crucial for learning distinct models. On its own, it requires training a very large number of models ($\gg$32) before picking up features outside the MNIST tiles. Visualizations of input gradients (Figure 6) reveal that these models each rely only on a single or a few pixels. These trivial solutions to the independence constraint, akin to adversarial examples, are avoided with the on-manifold constraint.
- In the full method ($\lambda_{\text{indep}} > 0$, $\lambda_{\text{manifold}} > 0$) the models discover distinct features that align with the semantic contents of images. The effect of the on-manifold constraint on input gradients is striking (Figure 6). It forces models to be sensitive to natural variations of the data – rather than unlikely single-pixel patterns. Remarkably, **image regions emerge as meaningful features without inductive bias for spatial locality** (*e.g.* no convolutions).

Hyperparameters. A number of models between 4 and 24 give excellent results. As expected, the larger this number, the more granular the features these models learn (Figure 6). The effect breaks down for >24 models, matching theoretical expectations since the dimensionality of the manifold was estimated at ∼24. The method is stable over a range of regularizer weights. Additional

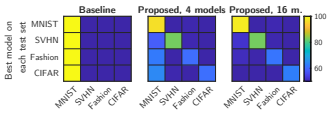
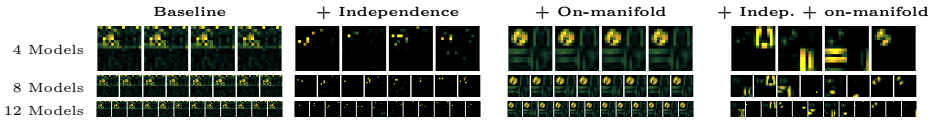


Fig. 5: Collages dataset: accuracy on the four test sets (columns) of models with best accuracy on each set (rows). Diagonal patterns indicate that **models specialize and learn different, non-overlapping features**. The baseline only learns features relevant to MNIST.



(a) With standard training, all models rely on a small, identical region of the image, despite the fact that predictive features are present all over.

(b) Independence produces distinct gradients, but many models are needed to discover new features and they are sensitive to isolated pixels.

(c) The on-manifold constraint forces gradients to align with natural variations of the data. Accuracy is virtually identical to the baseline.

(d) With both constraints, **we learn semantically relevant features in all image regions** with as few as 4 models.

Fig. 6: Input gradients for a random test image from the collages dataset. It is remarkable that, with the proposed method (d) **image regions emerge as meaningful features without any inductive bias for spatial locality** such as convolutions (models in these experiments are fully-connected MLPs).

comparisons in Table 1 show that a VAE is better than PCA to represent the manifold. This agrees with the general expectation that natural images form a non-linear manifold in pixel space. We also found overall results to be robust to variations in architecture and hyperparameters of the VAE.

Fine-tuning. We report the accuracy of models fine-tuned on masked inputs as proposed in Section 3.3. This optional step relaxes the independence constraint to maximize each model's predictive performance. The accuracy jumps significantly and almost reaches the upper-bound on each test set (Table 1). We experimented with relaxing both the independence and on-manifold constraints. Disabling the former has a significant effect. But the latter has no significant effect on accuracy on its own as expected and discussed in Section 3.2.

Distilling multiple models into one. We report the performance of combinations of features described in Section 3.4. This procedure is most effective after training a large number of models (24 here). This is unsurprising since models then discover finer-grained features. Each combination selects features relevant to only one specific tile to achieve near-maximal accuracy on the test set of that tile. Simple traditional ensembling of models completely failed in our experiments.

Comparison with existing methods. No other method reported in Table 1 performed well on this dataset. The method of Teney *et al.* [48] is technically the most similar to ours, but it requires training a much larger number of models and still achieves much lower accuracy. While all experiments of this section used a model taking raw pixels as input, we repeated the whole evaluation using a shared, frozen ResNet to extract features in the supp. mat. This implementation

is computationally appealing for larger-scale applications, and gave essentially similar findings with higher overall accuracy thanks to the deeper architecture.

Collages (accuracy in %)	Best model on				
	MNIST	SVHN	Fashion	CIFAR-10	Average
Upper bound (training on test-domain data)	99.9	92.4	80.8	68.6	85.5
ERM Baseline	99.8	50.0	50.0	50.0	62.5
Spectral decoupling [35]	99.9	49.8	50.6	49.9	62.5
Penalty: gradients' L1 norm	98.5	49.6	50.5	50.0	62.1
Penalty: g. L2 norm [18]	96.6	52.1	52.3	54.3	63.8
Input dropout (ratio 0.9)	97.4	50.7	56.1	52.1	64.1
Indep. loss (cos. sim.) [39]	99.7	50.4	51.5	50.2	63.0
Indep. loss (dot prod.) [48]	99.5	53.5	53.3	50.5	64.2
With many more models					
Indep. (cos. sim.), 1024 models	99.5	58.1	66.8	63.0	71.9
Indep. (dot prod.), 128 models	98.7	84.9	71.6	61.5	79.2
Proposed method (8 models)					
Indep. + on-manifold PCA	97.3	69.8	62.2	60.0	72.3
Indep. + on-manifold VAE*	96.5	85.1	61.1	62.1	76.2
(*) + FT (fine-tuning)	99.7	90.9	81.4	67.4	84.8
(*) + FT + combi. (1×)	99.9	92.2	79.3	66.3	84.4
(*) + FT + combi. (2×)	99.9	92.5	80.2	67.5	85.0
(*) + FT + combi. (3×)	**99.9**	**92.3**	**80.8**	**68.5**	**85.4**

Table 1: Accuracy on *collages* of existing and proposed methods (8 models per method unless specified). The 4 test sets simulate different OOD conditions: only one tile in each set is correlated with the labels. **Standard training only learns a fraction of predictive features**. Existing methods cannot do better than chance except on MNIST, or they require training a large number of models. Ours learns a variety of features and give near-optimal predictions on every test set (last row).

4.2 Experiments on real data: WILDS-Camelyon17

Dataset. The WILDS-Camelyon17 benchmark [26] provides histopathology images to classify as "*tumor*" or "*normal*". The images come from different sets of hospitals in the training, validation (val-OOD), and test splits (test-OOD). The challenge is to learn a model that generalizes from the training hospitals to those of the test set. The original authors [26] trained a Densenet-121 model from scratch on this data with 10 random seeds. They showed that the performance on val-OOD and test-OOD varies wildly across seeds, demonstrating that the task is severely underspecified with only the standard training images (the dataset provides additional hospital labels that could enable generalization; neither ERM nor our method uses them).

h **Implementation of our method.** We use frozen features (last-layer activations) from one of the pretrained models from [26] as input. We will show that we can recover even more variability in performance than the complete models trained on different random seeds, even while keeping the model frozen (*i.e.* retraining only a classifier). We first determined that the best ERM-trained classifier on frozen features is a simple linear one, rather than an MLP. Our method simplifies in two ways with a linear classifier. First, input gradients are equal to the classifier weights, and the proposed regularizers do not require second-order derivatives anymore during back-propagation. Second, we found empirically that the soft on-manifold regularizer can be replaced with a hard constraint: we explicit project the input gradients onto the manifold and apply the independence

WILDS-Camelyon17	Best accuracy (%) on val-OOD	test-OOD
Pseudo-Label [29]	–	67.7 ±8.2
DANN [9]	–	68.4 ±9.2
FixMatch [45]	–	71.0 ±4.9
CORAL [46]	–	77.9 ±6.6
NoisyStudent [56]	–	**86.7** ±1.7
ERM Baseline	84.9 ±0.1	68.4 ±0.1
+ Independence constraint	85.3 ±0.5	74.6 ±0.9
+ On-manifold soft regularizer, VAE	85.4 ±0.4	80.3 ±1.7
+ On-manifold hard projection, VAE	88.2 ±2.1	76.3 ±2.8
+ On-manifold soft regularizer, PCA	87.8 ±0.3	79.0 ±2.9
+ On-manifold hard projection, PCA*	**88.4** ±0.7	81.6 ±1.4
(*) + Fine-tuning & distillation	**88.4** ±0.7	**82.5** ±2.4

Table 2: Accuracy on WILDS-Camelyon17 while training 12 models. Each proposed component improves the accuracy of the best model from each run. The data appears simple enough that a PCA approximates the manifold well enough. This allows implementing the on-manifold constraint as a hard projection instead of a soft regularizer.

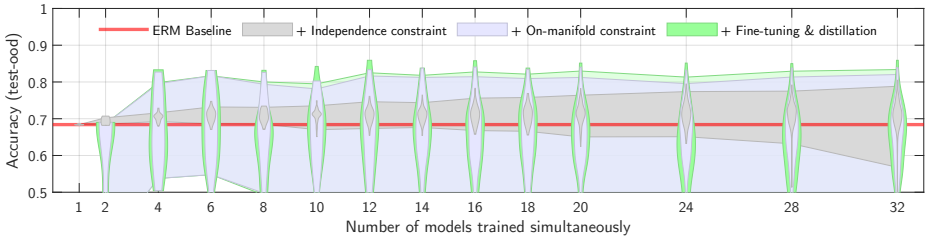


Fig. 7: Spread of accuracies on WILDS-Camelyon17 of models trained with different ablations of our method. The upper/lower bounds of the **shaded areas** show the highest/lowest accuracy of any model from one run, averaged over 6 seeds. The **violins** show distributions of accuracies over *all* seeds (hence some values outside the shaded areas). The independence constraint (**gray**) produces a wide variety of models, as opposed to the baseline (**red** line). However, the highest accuracy in each run grows slowly with the number of models. With the on-manifold constraint (**blue**), the improvement is larger and requires fewer models. Fine-tuning/distillation (**green**) bring additional marginal improvements.

regularizer on these projections, as proposed in [39]. As noted in Section 3.2, this option completely failed in our early experiments with MLPs, but it seems viable with linear classifiers. This further simplifies the implementation.

Results. We plot in Figure 7 the spread of accuracies of models trained with different methods (using features from the first pretrained model from [26], see the supp. mat. for similar results with the others). The **ERM baseline** simply recovers the accuracy of the original complete Densenet, with essentially no variation across random seeds. With our **independence constraint**, the spread of accuracies significantly widens, both below and above the baseline. In the supp. mat. we show that the models span various trade-offs in accuracy on val-OOD and on test-OOD, neither of which is correlated with the accuracy on in-domain data (val-ID), thus showing evidence of underspecification. Back to Figure 7, with our additional **on-manifold constraint**, the best models reach higher ac-

curacies. This also tops out when training a handful of models (about 10–14, near the intrinsic dimensionality of the data estimated at 12 with [37]). Keeping in mind that we use frozen features, these results show that the ERM-pretrained model extracts features useful for OOD performance but that are ignored by the pretrained classifier. Similar findings were recently reported in [25,38]. Our method recovers these features and produces alternative classifiers with a variety of trade-offs in performance across various OOD conditions.

Ablations. In Table 2, we compare additional ablations of our method, using a fixed number of 10 models. The **essential components are the independence and on-manifold constraints**. The fine-tuning and distillation steps contribute to a marginal improvement. We report similar *relative* improvements in the supp. mat. with other pretrained models, but the absolute performance is very much **dependent on a "good" pretrained model**.

Model selection. Our method brings similar relative improvements on either val-OOD or test-OOD but typically with different models for each (see Figure 7) despite both being OOD relative to the training data. **Model selection absent labelled target-domain data therefore remains an issue** on this dataset. Fortunately, only little such data may be sufficient. We repeated a few experiments while holding out 1% of test-OOD (less than 1,000 instances) and we observed a 99.87% correlation coefficient between the accuracy on test-OOD and this held-out data. While all our results assume perfect "oracle" model selection, it seems reasonable that real applications could provide a small amount of labelled test data to achieve similar results.

5 Discussion

We presented a method that highlights cases of underspecification by training multiple models with similar in-domain performance yet different OOD behaviour. This method offers a partial solution to building robust models since it discovers features that are otherwise missed by standard ERM due to shortcut learning or other implicit inductive biases [33,43].

What do we gain from identifying cases of underspecification? The level of underspecification (indicated by the number of models that can be trained with the proposed constraints) shows how far from unique a solution to a learning problem is. Diagnosing underspecification is not a pass-or-fail test: all but the simplest tasks and models are underspecified to some extent. Measuring underspecification should help determining the level of trust attributed to an ML model. Our constructive approach has the added advantage of exposing the range of predictive features present in the data.

Importance to both engineering and science. There is a continuing source of research questions in the apparent mismatch between empirical practices in ML and some hard limitations of learning methods. The concept of underspecification has the potential to unify phenomena including shortcut learning, distribution shifts, and adversarial robustness. These are important for ML as an engineering discipline (improving reliability and applicability of ML methods)

as well as a scientific endeavour (understanding the structure of real-world data and how/why existing methods work).

A first implication of underspecification is that ERM is insufficient to guarantee OOD generalization. Identified cases of underspecification point at the need for additional task-specific information in the design of reliable learning methods. If such information cannot be integrated, learned models are at risk of unexpected behaviour when deployed on OOD data, because the depend on stochastic or arbitrary factors (*e.g.* texture *vs.* shape in image classification [12]).

A second implication is that ID and OOD performance are not necessarily coupled. Without further assumptions, in-domain validation is not a reliable model selection strategy for OOD performance despite some suggestions *e.g.* in [16,31]. It might be useful as a heuristic owing to some inherent structure in real-world data, but its limits of applicability are yet to be understood.

A third implication is that high OOD performance of a model is no guarantee for its reliability. High apparent performance might happen by accident in an underspecified setting. In such cases, the model behaviour depends on hidden assumptions and it could still fail unexpectedly. Identifying underspecification remains important to identify these hidden assumptions, which is particularly important for high-stakes applications such as medical imaging [3,13].

The proposed analysis also corroborates existing explanations for techniques that successfully improve generalization, such as data augmentation and contrastive learning. Both were indeed shown to depend on the injection of additional knowledge, respectively in the design of the augmentations [4,21,28] and pair selection strategy [57]. And this extra knowledge is often task-specific [55]. For example, augmenting images with rotations may help in identifying flowers but not traffic signs. Injecting task-specific knowledge is sometimes vilified in a "data-driven" culture. This study suggests that we would rather benefit from highlighting this practice and making assumptions more explicit, thus helping one to identify the limits of applicability of various methods.

Conclusion. This paper made theoretical and methodological steps on the study of underspecification. It complements an observational study [6] with a method to diagnose and address the problem.

Limitations. The proposed method for building models with better generalization is only a partial solution since it requires an external model selection procedure. New methods for model selection [8,11,22,52], robust evaluation [10,23], and explainability [14,49] are all suitable to implement this selection. Interactive approaches [7] are another option that injects expert knowledge. Another possible extension is to apply the method to the end-to-end training of larger models. Finally, this work focused on i.i.d. training data. We hope to extend the analysis to forms of data known to be valuable for OOD generalization such as multiple environments [2,34,5], counterfactual examples [23,47], and non-stationary data [1,17,36,51]. The analysis of multi-environment training as used for domain generalization may elucidate why these methods often fail in practice [16].

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