Abstract

It is prevalent and well-observed, but poorly understood, that two machine learning models with similar performance during training can have very different real-world performance characteristics. This implies elusive differences in the internals of the models, manifesting as representational multiplicity (RM). We introduce a conceptual and experimental setup for analyzing RM and show that certain training methods systematically result in greater RM than others, measured by activation similarity via singular vector canonical correlation analysis (SVCCA). We further correlate it with predictive multiplicity measured by the variance in i.i.d. and out-of-distribution test set predictions, in four common image data sets. We call for systematic measurement and maximal exposure, not elimination, of RM in models. Qualitative tools such as our confabulator analysis can facilitate understanding and communication of RM effects to stakeholders.

1 Introduction

Machine learning models are typically underdetermined by data, which is often poorly understood, imprecisely conceptualized, and only superficially measured. Consequently, it is easy to mistake the observed success of a model for proof that it has somehow ‘captured’ the relevant features of its target. This oversight, in turn, leads to surprising practical problems with real-world model generalization. As ML models are increasingly deployed into real-world environments, it has become common to find that a model that worked well in the tests faces various failures in real-world scenarios. The textbook explanation for this disconnect is that the training data of the model and the deployment-time data were not generated from the same distribution (‘non-iid’). In that case, the model that appeared best during the training simply does not fit the relevant data, rendering the predictions unreliable.

Our focus here is on the more elusive yet prevalent case in which multiple variants of a model that perform equally well with training data will perform very differently from each other on new (unseen during training) test data. Here, the data available at training time is simply insufficient to justify sound model selection among the model variants. This phenomenon has been approached with concepts such as non-identifiability, underspecification [1], Rashomon set [2, 3], arbitrariness-1 [4], and predictive multiplicity [5]. While the resulting model selection problem appears well-grounded in data analysis [6], the established techniques assume a well-defined likelihood measure, which in case of neural networks often does not exist.

Hence, we have risk-equivalent model variants that internally represent the same data differently. We call these postulated internal differences across the model variants representational multiplicity (RM). These differences, in turn, bring about the observed spread of predictions across the variants of the same model, the definition of predictive multiplicity (PM, [5]).

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In practice, the multiplicity may be brought about by seemingly random factors like “the particular scheme used for initialization; conventions for parameterization; choice of optimization algorithm; conventions for representing data; and choices of batch size, learning rate, and other hyperparameters, all of which may interact with the infrastructure available for training and serving models.” [7]. Technically, underspecification is always possible for large models [1]. It limits the reliability of inferences for explanatory purposes and seems to undermine the very notion of a ‘best model for the data’. Multiplicity, like non-identifiability in statistics, may or may not involve uncertainty about the underlying causal structure of the data.

Since variations in predictive outputs logically require variance in the intermediate representations, the presence of PM implies the presence of RM. The opposite is not the case, since, for a given sample, two different representations can still lead to the same prediction. PM only measures the observable predictive differences as a function of the test samples at hand, within the limits set by RM. Even in absence of observed PM, any presence of RM implies that there exist other potential inputs that would also yield observable PM. We construct an experiment to demonstrate this (Fig. 2).

Many prior works approach the phenomenon via elimination or reduction to uncertainty. The elimination of the problem can be defended if one can plausibly unearth the underlying causal properties via designing a set of interventions to that end (see D’Amour et al. [1] for a large scale empirical evaluation, Romeijn and Williamson [8] for theoretical analysis). Yet, this rarely happens in ML modeling except in the very theory of causal inference itself (e.g. see Schölkopf [9]). In Bayesian and ensemble analyses (e.g., [10–12]), the variance is characteristically treated in aggregate, usually in parameter space. Finally, as a matter of standard ML practise, the variance is reduced to a scalar for generalization error, even in the in-depth analysis of the topic in Raghu et al. [13].

In contrast, we approach RM as a fundamentally irreducible phenomenon for a given model family. Observed RM is taken to amount to information, not noise. This leads us to focus not on how to mitigate RM, but rather on how to expose it. For a given observed performance level of a model, we argue that the observed extent of RM should be maximized rather than minimized, as the opposite approach would encourage overestimation of the generalisation power of the model.

This led us to investigate whether there are systematic relationships between certain training strategies and the magnitude of RM. It has been observed, for instance, that a specific learning rate tends to pick a cluster of similar variants [13, 14], but systematic analysis of whether certain training strategies cause more RM than others has so far been lacking. Our results in vision data sets not only confirm considerable RM across random seed selection, but also indicate that the relative degree of RM is strongly correlated with (inverse) batch size and learning rate. Furthermore, irrespective of the well-known association between larger batch sizes and worse generalization via sharper minima[15–17], we observe a strong connection between larger batch sizes and lower variance in predictions across model variants, that is, lower predictive multiplicity (PM). As far as we are aware, this is also the first attempt at evaluating the connection between RM and PM.

Our emphasis on RM aims to raise questions about the discourse based on a one-dimensional notion of ‘the best’ model for the data, and equivalent-sounding notions like ‘predictor that encodes the right structure’ [1], ‘[models that contain] the true data generating process’ [3] or even ‘true data generating model’ [6]. This terminology suggests one can cross and dissolve the categorical gap between the model and the modeled. However, in the general case, representational multiplicity can only be hidden, not eliminated.

We summarize the contributions of this paper as follows.

- We present a conceptual and experimental setup for analyzing the critical and undervalued phenomenon of representational multiplicity (RM)
- We show various regularities between hyper-parameter selection and RM
- We justify the significance of observing both representational and predictive multiplicity, supported by experiments
- We introduce the confabulation matrix as an illustration of our approach
2 Related Work

The phenomenon of representative multiplicity in ML models is strongly related to well-known long-standing questions in, for example, underdetermination of theories in philosophy of science and epistemology, and system non-identifiability in statistics and economics. While there is extensive historical discourse on the matter, the implications for modern very large computational models are less obvious.

From this modern standpoint, the seminal paper by Breiman [2] focuses on the danger of overestimating the explanatory power of models, by highlighting the chasm between two conception of models. First, the models that are structurally designed and selected for explanatory purposes, and second, the models optimized for prediction. Under the latter paradigm, the data then admits several equally valid model parametrizations and ensuing explanations. These model variants constitute the Rashomon set.

In computer science, beyond the obvious connections to generalizability and overfitting, the problem has been approached at least in the context of loss landscape analysis (e.g., [18, 12, 19, 20]), overparametrization (e.g., [21]) model averaging (e.g., [12, 22]), domain adaption and interpretability, and ensembling [23, 11]. Risk-equivalent modes have also been examined from the point of view of accuracy-diversity tradeoffs ([11]) as well as accuracy-reproducibility trade-offs ([24]).

During recent years, empirical consequences of multiplicity have been examined in pathological cases such as spurious correlations and shortcut learning [9, 25]. D’Amour et al. [1] examines the prevalence and consequences of multiplicity in practical ML pipelines that admit ‘underspecification’. These works highlight that, often, there is simply not enough information in the training setup to guide the creation and selection of models so that they could confidently capture the most relevant inductive biases of the problem.

Underspecification and Rashomon sets have directly been leveraged in [26] with the goal of selecting models within the set, based on criteria such as sparsity or monotonicity along an important set of features. In a similar vein, multiplicity can also be leveraged to estimate variable importance [3].

The alternative notions of ‘underspecification’, ‘identifiability’ and Rashomon sets are closely related to the same scenario. To capture the internal and external aspects of the problem, the notion of representational multiplicity (RM) was introduced in this work to supplement predictive multiplicity (PM) introced in Marx et al. [5]. Prior works often do not explicitly discuss this distinction. Further, our PM definition accounts for the actual variance of predictions, whereas, for instance, D’Amour et al. [1] only measures multiplicity in image domain as the variation in total accuracy. Such aggregation actually ignores the distribution in the kinds of errors the model variants make.

Despite the usefulness of the ‘underspecification’ concept, the very notion is problematic for large models because it admits a possibility of ‘full’ specification, if only we try hard enough. The suggested approach in D’Amour et al. [1] is to introduce the notion of ‘credible intuitive bias’ as a target, which, if integrated into the training pipeline, would make this target stand out and thus, by definition, eliminate the underspecification. This advice may be valuable in terms of segmenting the ML workflow, but it appears circular: we ‘solve’ underspecification – originally defined in terms of unobserved downstream environment – by improving our pipeline so as to deal with the observed problems. Conceptually, this move merely shifts previously unobserved issues into the realm of observed issues, and solves them. It does not exhaust the realm of remaining unobserved issues.

Principled approaches to model selection exist in Bayesian statistics, with methods such as BIC and AIC routinely used to compare models. However, in practise, they are not applicable to deep neural networks [6] that perform equally well on the test data set. The same holds for techniques such as majority voting or randomization procedures [27].

Prior works that focus on mitigating the multiplicity in practise [1, 25, 9] are valuable as long as we can assume that the information is available to resolve the multiplicity. Our work considers the general scenario in which we have no way of knowing whether this is the case nor of distinguishing one model from another, which renders all RM variation informative. Following the same line of reasoning, while it may be useful to marginalize over all model variants in parameter space [22], that may risk throwing away relevant information.

To this end, the quantification of RM in the network activation space is critical, and effectively amounts to assessing network similarity. Here, we have chosen the SVCCA [13] which allows for
Figure 1: Associating representative (RM) and predictive (PM) multiplicity in two hyper-parameter regimes (Left: learning rate, Right: batch size) for three datasets, with identical model architectures. SVCCA is the measure of inverted RM at two feature layers, while the prediction ‘std’ columns measure PM for the i.i.d. and various OOD distributions. Datasets: FashionMNIST (top), CIFAR-9 (middle), and MNIST (bottom). Low learning rate and high batch size strongly correlate with higher SVCCA (lower RM) and smaller variance (lower PM).

efficiently comparing the similarity of distributed representations in different networks. SVCCA was demonstrably capable of even comparing different architectures as well as surfacing detailed learning dynamics, such as the order in which the layers ‘solidify’ during learning. Kornblith et al. [28] improve the reliability of the method when the number of evaluation data points is small.

The treatment of predictive multiplicity (PM) in [5] is closest in spirit to our work (but also see ‘Prediction variation’ metric in Chen et al. [29] and related Dusenberry et al. [30]). They call for exposing PM in quantitative measurements, and reporting it in the same way as the canonical test error. However, while they build upon ‘the Rashomon effect’ (effectively equivalent to RM), they focus on the practical consequences for predictions and do not quantitatively address the PM-RM distinction. Our work provides a more complete yet concise picture that draws from the methodology of [1], the explicit metrics for RM from [13] and the conceptual import for PM from [5]. Most importantly, we hope to expand the regular methodological approach in ML to incorporate these conceptual distinctions.

3 Methods

Problem Setup  We start with the classical setup for a supervised prediction problem, in which one aims to learn a function \( h : \mathcal{X} \rightarrow \mathcal{Y} \), i.e., \( h \) is the loss function \( \ell \) based on a training set \( \mathcal{X}_{\text{train}} = \{x_i\}_{i=1}^N \). The test data \( \mathcal{X}_{\text{test}} \) is a subset of the same distribution and satisfying the common i.i.d. assumption.

Predictive Multiplicity  Let \( H = \{h_k\}_{k=1}^K \) be a set of classifiers such that \( E(h_k) = E(h_j) < \epsilon \) for all \( h_k, h_j \in H \) with \( k \neq j \) and a given error tolerance \( \epsilon > 0 \). We define Predictive Multiplicity (PM)
over a data set $S$ and $H$ as: $PM(S, H) = \mathbb{E}_{x \in S}\left[\sqrt{\text{Var}_{h \in H}\{h(x)\}}\right]$. In words, we measure the extent to which the risk-equivalent model variants assign conflicting predictions over the dataset. Note that while we follow the concept definition of Marx et al. [5], we diverge from their mathematical definition.

**Representational Multiplicity** Representational multiplicity can be defined in three components. First, it is a measure of variation across the internal representations of risk-equivalent models, defined in terms of certain empirical risk. This is in contrast to the variation in predictions. The representations are expressed by activations in the function space. Unlike evaluation in the weight space, the (function) activation space yields a similarity estimate informed by the available data. Hence, we focus on dissimilarities between the learned functions rather than their parametrization. The latter can be diverse even if the underlying functions are not [18]. Second, the multiplicity and risk must be defined in terms of specific data, typically the training or testing data already available in the context. Third, the relevant variation across the representations must be asymmetric in terms of trivial transformations such as affine transformations. In practise, the latter constraint prevents us from, for instance, mistaking two neural network representations as different when the difference is merely due to the different order of the same weights in latent space. Importantly, this excludes the use of straight-forward measures such as standard deviations in the activation space.

A suitable approach is the singular vector canonical correlation analysis (SVCCA) metric [13], a method for assessing activation similarity via combining Singular Value Decomposition with Canonical Correlation Analysis (CCA) [31]. When comparing two activation vectors, first, SVCCA performs SVD on both, to compute the most relevant directions in their respective subspaces. Then, it computes the Canonical Correlation similarity by transforming the subspaces in a way that maximizes their mutual correlation. Since CCA is invariant to affine transformations, the method is well-suited for RM estimation.

$RM(S, f)$ is then defined as the mean of the coefficients of the first 20 SVCCA vectors which constitutes a single similarity measure for dataset $S$ and (sub-)network $f$. For SVCCA among more than two network variants, we paired every variant with each other and took the mean of the triangular matrix produced by all the pairings. We considered SVCCA separately for each model’s last CNN layer ("cnn") and the first fully connected one ("fc1").

**Assessing Patterns in RM and PM** Let us now pull together the steps needed to assess the patterns in RM and PM. First, we are interested in the individual predictions for each $x_i$ in the data set, as opposed to looking at their aggregate error. We need them since, once we train all $h_k \in H$, $k = 1, \ldots, K$ variants of this model (changing nothing but the random seed), we thus receive the variance of predictions separately for each $x_i$ across the variants in $H$.

To understand why, consider an example with two training strategies A and B. Assume that each training run yields 99.0% accuracy, but when we look at the variance of predictions across model variants, for each separate input, and take the mean, strategy A turns out to yield far higher variance than strategy B. This is PM, informing us that the behavior of the two cases is very different. Then, separately for A and B, the mean SVCCA of each $h_k$ against each $h_j$, $j \neq k$ measured on the full data set yields us RM.

Finally, we can select a hyper-parameter $\alpha$ (‘regime’) for $M$ different values of it (‘strategies’), we measure PM and RM, and repeat the PM for various OOD test sets. For each regime, we can now track whether one strategy yields higher PM or RM than another. Finally, we can compare the whole regimes of learning rate and batch size and look for similarities.

To compare variants of the same model, we must stop the training in each case once we reach the predictive accuracy that we presume can be achieved by all the variants and hyper-parameter values.

**Primacy of RM** Consider the decomposition of a multi-layered neural network function $h$ into $h = f \circ g$, for various potential splits between $f$ and $g$. RM is measured at the output layer that defines the $f$, leaving a non-trivial $g$ consisting of one or more layers. Let us now consider the case where $RM(S, f) = 0$ for the set of model variants $f \in F$, and data set $S$. This would imply that $f_k(x) = f_j(x)$ for all $k \neq j$. Given that PM is defined in terms of the set $H$, it is evident that $PM(S, f_k \circ g_k) = PM(S, f_0 \circ g_k)$. Hence, if $g_k$ is deterministic, we would have $PM(S, h_k) = 0$ for all $k$. Vice versa, if $PM(S, h) > 0$, it necessarily follows that $RM(S, h) > 0$. Hence, the presence of PM implies the presence of RM, but not necessarily vice versa.
Figure 2: Relevance of RM. We compare the predictive power of RM vs. PM in two datasets under two hyper-parameter regimes, each. In order to show that there exist cases where RM cannot be reduced to PM, we first select a subset of 1000 samples for each dataset such that those samples have the lowest overall PM. For each strategy (7 different descending learning rates or increasing batch sizes), we then plot the PM-1k of those 1000 samples for each strategy (red), the actual final PM after observing all 10k or 26k samples (blue), and the RM-1k computed from the same subset of 1000 samples. This comparison surfaces the strong correlation between RM-1k and the PM of the full dataset, whereas the PM-1k and the PM of the full dataset are uncorrelated. This confirms the intuition that, over a small sample with very little observed PM, RM can be superior to PM in predicting the final PM that will become observable with a larger sample.

**Arbitrary Predictions** In the traditional best-model based analysis of classification models, it is common to review which samples are most prone to classification errors with that model, often presented as a confusion matrix. Now, admitting the possibility of RM, one can similarly ask which samples are most prone to being differentially classified across various equally accurate variants of the model. This yields a sort-of ‘second-order’ confusion analysis that we call **confabulation analysis**, visualized in terms of the inputs that yield the highest multiplicity values (Fig. 3).

The terminology is motivated by the fact that the choices the model makes for those samples appear arbitrary, or conFabulated, irrespective of how confident a specific model instance is about them.

There is a major conceptual difference between confusion and confabulation. Confusion is about what kind of samples our model is currently wrong about, suggesting we should do something about it. Confabulation is about the kind of samples our models might be fundamentally unable to classify correctly, so ambivalent or devoid of relevant information that they should perhaps be discarded altogether.

In a disturbing contrast, the common approach to force one’s model to classify even the worst of these samples “correctly” may be akin to learning to classify noise.

**4 Experiments**

We conduct three types of experiments to support our case. First, we examine the relationship between RM and PM in various datasets, and see how they relate to out-of-distribution (OOD) generalization, under various training scenarios. Second, we focus on the distinction between RM
and PM measurements, showing that one cannot simply reduce RM to PM. Third, we visualize the concrete manifestations of high RM.

**Data Sets and Architectures**  In order to examine the representational multiplicity in classifiers with typical small vision data sets, we trained classifiers on four sets of small images: MNIST, FashionMNIST [32], CIFAR-9 (CIFAR-10 [33] with one dropped class), and SVHN [34]. We used SVHN as an OOD dataset for MNIST and STL9 (STL10 [35] with one dropped class to match CIFAR-9) as an OOD data set for CIFAR-9. Our focus was on typical scenarios, so for each data set, we picked a simple CNN architecture and controlled for the same reasonable but not state-of-the-art accuracy within the dataset (see Supplement B for training details).

**Peculiar Regularities in Training Strategies**  Our approach was to consider the relevant measurable differences in risk-equivalent (i.e., equally accurate) models trained with the same data, model structure, training strategy, and other hyper-parameters. The baseline assumption was that such model variants should be, effectively, behaviorally equivalent.

To measure the empirical divergence from this assumption, for a single strategy, we first keep all hyper-parameters the same, and train 10 variants while only changing the random seed. We then measure the SVCCA similarities and variance of the outputs, separately for manual augmentations that transform the dataset to OOD and for the matching separate OOD datasets. In fig. 1, this represents a single continuous line. We then consider the effect of the training strategy by trying 7 values for each hyper-parameter regime, and repeat the measurements. We repeat this separately for batch size and learning rate (but we could have included other things such as initialization, optimization parameters, etc.). This yields $2 \times 7 \times 10$ training runs per dataset (the 7 continuous lines).

To ensure that the results within each dataset are risk-equivalent, we first had to determine the maximum (test set) accuracy that can be reached using any of the hyper-parameter values in the tested range. For the actual training sessions, we then stopped the training in each case at this value. Following the training to the highest achievable accuracy would not have made a difference to the conclusions (see Supplement C).

The interesting patterns to look at are, for each line, whether there are suspiciously small SVCCA (high RM) and large i.i.d. test set prediction variance (high PM) values, whether the two are correlated, and how they relate to the OOD prediction variances. Across the lines, the first interesting question is whether they coincide, and if not, how widely dispersed they are. This informs us about whether the hyper-parameter affects the multiplicity of potential solutions. For instance, even without knowing whether SVCCA value of 0.3 is “low” or not, it certainly seems relevant that some learning rates yield 0.3 and some 0.6. Finally, we look at whether the magnitude of the varied hyper-parameter is directly correlated with the magnitude of the ensuing PM or RM.

Across the data sets, our results point to clear correlations between the strategic parameter (batch size or learning rate) and RM. The larger batch size and the smaller learning rate correlate strongly with higher SVCCA similarity in both the last CNN and the FC1 layers (Fig. 1). Moreover, both correlate strongly with smaller PM both in the i.i.d. test set and OOD test sets. (For more experiments, see Supplement fig. 4.)

Of the four data sets included, a clear exception was observed with MNIST under the batch size strategy, which showed the most distinct behaviour. This is likely due to the small range in SVCCA values, especially since MNIST with the LR strategy, with a wide SVCCA range of $[0.737, 0.849]$, shows the same regularities as observed with other data sets (Fig. 1). As an alternative to SVCCA, we also attempted the CKA metric [28] for the same purpose, but failed to observe any correlation between CKA and PM values, hence we chose not to use it for the analysis.

Measurements of Pearson correlation coefficient (Table 1) across datasets support the same conclusions.

**Relevance of RM as Predictor**  Given the correlations between RM and PM, one might well ask, do we really need RM in the first place, when PM often appears to be more easily accessible? Conceptually, RM must necessarily precede PM, but at the limit of infinite test data, all the interesting variation in RM must necessarily be perceived as PM. On the other hand, under limited data, some of the internal variation (RM) will still be collapsed at the final layers, at least under operations such as softmax activation. Hence, to demonstrate the difference empirically, one can simply construct the existence proof for a case where the two are not equivalent.
Figure 3: Top-16 confabulation inputs for CIFAR-9, SVHN, FashionMNIST, and MNIST. Confabulation measures the diversity of predictions assigned to each sample, across different training runs of the same model. In other words, the highly confabulated items are those that will most likely be classified differently under different runs. This is more informative a measure than the aggregate classification error. Considering some of the numbers, for instance, it is evident that forcing the model to learn their "correct" class amounts to learning noise.

Table 1: The Pearson correlation coefficient (PCC) between negative representational multiplicity (RM) measured using SVCCA metric, and predictive multiplicity (PM) measured using standard deviation between OOD predictions across the data sets (LR = learning rate). The columns 'x-flip' (horizontal flip), 'Pixelate' and 'Coloring' represent the OOD predictions, followed by exposition of the range of RM values for the dataset and the strategy ($\Delta$ SVCCA). Strong negative correlation values indicate that PM and RM align.

| Data set | x-flip | Pixelate | Coloring | $\Delta$ SVCCA (fc1) |
|----------|--------|----------|----------|-----------------------|
| F-MNIST  | −0.750 | −0.991   | −0.872   | −0.767 −0.978 0.037 0.301 |
| CIFAR-9  | −0.623 | −0.990   | −0.571   | −0.609 −0.985 0.073 0.445 |
| SVHN     | −0.422 | −0.986   | 0.191    | 0.089 −0.985 0.033 0.234 |
| MNIST    | −0.482 | −0.977   | 0.221    | 0.063 −0.932 0.041 0.167 |

To this end, we first measured the PM for a full training dataset for Cifar-9 (10,000 samples) and SVHN (26,000 samples). Then, we picked a subset of 1000 samples with the lowest PM, as these items are likely to yield the least amount of information about RM. Using the same samples, we measured RM. Finally, we asked, is the PM or RM in the 1k sample predictive of the PM for the whole dataset, when measured for different training strategies? As seen in in Fig. 2, after scaling all values to $[0, 1]$ range, the RM values for the 1k subset are strongly correlated with the PM values of the whole dataset, whereas the PM of the 1k test set are uncorrelated. Note that the 1k sample was in no way selected to favor the utility of RM values as such. Hence, we have shown that the information captured by RM about the data is not reducible to the information captured by PM alone.

Confabulator Inputs  We visualize the confabulation matrices in Fig. 3 for all data sets. The confabulators appear similar to what one might expect in confusion matrices, but here, they reflect not just a single training run, but a range of independent sessions. (Note that the confabulations are computed across all training strategies, and could further be examined for each recipe separately.)

5 Conclusion and Limitations

We propose exposing the representational multiplicity reachable in a given ML problem setup. As a preliminary example, considerable representational and predictive multiplicity appear in all four data sets studied. Within the network architectures considered, certain choices of basic training hyper-parameters appear to correlate with higher occurrence of multiplicity. Given the apparent ubiquity of these phenomena, we suggest that, in general, model evaluation should either include such measures or explicitly address their absence, so as to not overstate the power of the resulting models.

The prevalence of RM raises questions about the ML practises and discourse based on the one-dimensional notion of ‘the best’ model for the data, and its equally imaginary counterpart ‘unbiased
model’. Thus construed, ‘the best’ appears as if it should transcend the model–data gap altogether and, in some unconditional sense, capture the objective patterns in the data. It is as if the categorical difference between the model and the modeled gets blurred into a mere difference of degree. Any failure to cross the often-impossible chasm then leaves room for ethical questions in the form of biases that cannot be resolved.

The experiments heavily rely on using the top 20 SVCCA vectors as a proxy for negative RM. While the observed regularities lend credence to this decision, the search for and comparison of different proxies for RM is an interesting path forward.

This study was limited by the characteristically extensive need for computational resources for over 500 training runs. We only looked at classification models, which likely behave very differently from, for instance, generative models. Large image data sets and architectures were thus not examined. Only two training strategies were compared, and we did not study the effects of normalization strategies or different optimizers (ADAM [36] was used). While these limitations indicate that a larger research effort is called for, our key results are sufficiently consistent across four separate data sets so as to serve as a starting point for follow-up studies.
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A Extended Results

![Graphs showing comparisons for different datasets](image)

Figure 4: More comparisons of representative (RM) and predictive (PM) multiplicity, with SVHN dataset included to showcase that SVHN in learning rate regime breaks some of the trends observed with other datasets. Two hyper-parameter regimes are shown (Left: learning rate, Right: batch size) for four datasets. Identical model architectures were used for every hyper parameter of a dataset. SVCCA is the measure of inverted RM at two feature layers, while the prediction ‘std’ columns measure PM for the i.i.d. and various OOD distributions. Datasets: FashionMNIST (top), CIFAR-9 (middle), SVHN, and MNIST (bottom). Low learning rate and high batch size strongly correlate with higher SVCCA (lower RM) and smaller variance (lower PM).

B Training Details

Architectures We trained MNIST, SVHN and FashionMNIST with the typical convolutional architecture \( \text{conv}(1,48,3) - \text{ReLU} - \text{MaxPool}(2,2) - \text{conv}(48,96,3) - \text{ReLU} - \text{MaxPool}(2,2) - \text{conv}(96,80,3) - \text{ReLU} - \text{conv}(80,96,3) - \text{ReLU} - \text{FC}(96,512) - \text{FC}(512,10) \) and Cifar9 with \( \text{conv}(3,48,3) - \text{ReLU} - \text{MaxPool}(2,2) - \text{conv}(48,96,3) - \text{ReLU} - \text{MaxPool}(2,2) - \text{conv}(96,80,3) - \text{ReLU} - \text{conv}(80,96,3) - \text{ReLU} - \text{FC}(384,512) - \text{FC}(512,9) \).

Training Apart from the architecture, the same training methods and hyper-parameters were used for each dataset and run, with the exception of the batch size and learning rate. In learning rate regime, we used batch size 64 while using the learning rates...
Table 2: Test set accuracy statistics for the data sets used in this work.

| Dataset (HP regime)           | Mean ± Std   |
|------------------------------|--------------|
| CIFAR-9 (batch size)         | 0.709 ± 0.001|
| CIFAR-9 (learning rate)      | 0.643 ± 0.005|
| FashionMNIST (batch size)    | 0.940 ± 0.007|
| FashionMNIST (learning rate) | 0.930 ± 0.015|
| MNIST (batch size)           | 0.979 ± 0.001|
| MNIST (learning rate)        | 0.981 ± 0.002|
| SVHN (batch size)            | 0.905 ± 0.001|
| SVHN (learning rate)         | 0.894 ± 0.002|

[0.003, 0.002, 0.001, 0.0003, 0.0001, 0.00003, 0.00001]. In batch size regime, we used learning rate 0.0001 and batch sizes [8, 16, 32, 64, 128, 256, 512]. Cross entropy loss was used, with ADAM optimizer ($\beta_1 = 0.9, \beta_2 = 0.999, \epsilon = 1e^{-08}$).

For each dataset, we first found the maximum test set accuracy comfortably achieved by every strategy for each hyper-parameter regime of that dataset. We then trained 10 variants for each of them, varying only the random seed between the runs. We then used the checkpoints at the target levels for our evaluations. The accuracies were reached as in table 2. Note that it was not our goal to achieve state-of-the-art accuracy for the experiments of this paper.

**Datasets** MNIST, FashionMNIST, SVHN, and CIFAR-9 were used for training. STL-9 was additionally used as an extra OOD test dataset. CIFAR-9 was made by dropping the class ‘frog’ and STL-9 by dropping the class ‘monkey’, after which the class order of the two sets was made to match so that STL-9 served as the OOD dataset for CIFAR-9 trained models. The standard training/validation split was used for each dataset. Note that since we explicitly focused on our specific hyper-parameter strategies, there was no need for a separate validation and test datasets, hence, for each dataset, the held-out data was treated as the i.i.d. ‘test’ data.

For out of distribution (OOD) datasets, we cross-matched datasets as SVHN against MNIST, and CIFAR-9 against STL-9. In addition, other OOD datasets (see Fig. 1) were created from the original datasets in the following manner. The ‘x-flip’ was created by random horizontal flip with .9 probability, ‘color jitter’ by randomly changing brightness uniformly with a factor 0.0 to 0.3 and hue by a factor $-0.1$ to $+0.1$. Pixelation was done by downscaling and upsampling by a factor of 2. ‘OOD rot’ refers to rotations done to the original dataset by uniformly random increments of 0...20 degrees, 20...30 degrees, etc., up to 90...110 degrees, to yield 10 OOD test cases. The ‘min std’ and ‘max std’ in the figure refer to smallest and the largest rotation range, respectively.

The datasets contained no person identifiable data. All the datasets allow non-commercial usage for research purposes.

C Training to Maximum Accuracy

We take as a given that there are less model variants that achieve the top performance than there are variants that achieve sub-par performance (for empirical comparisons, see Fort 2020). In other words, the increase in validation accuracy should correlate with decreasing diversity of possible solutions.

One should then ask, first, is it possible that the decreased diversity of solutions reached by some hyper-parameter strategies can be explained by the greater achieved accuracy? By controlling for the test accuracy across compared variants (Fig. 1), we preclude this explanation.

Second, one can further ask, whether the differences could still be explained by the greater achievable accuracy, that is, perhaps there is less diversity with the solutions that are on the right path to achieve maximum accuracy? Though the hypothesis appears contrived, we addressed it by checkpointing but not stopping the main experiments at the equivalent-risk level. Instead, we also followed each experiment until convergence, and identified the pseudo-maximum accuracy for each training strategy, so that the maximum accuracy was achieved in at least 5 of the runs. (The absolute maximum accuracy would of course, strictly speaking, be only achieved by a single variant, preventing any dispersion analysis.)
In Fig. 5, we show the same results as in Fig. 4, but measured for the variants that achieve the pseudo-maximum accuracy for that strategy. Although one can see some repeating patterns, the decreased diversity of solutions certainly does not correlate with greater achieved accuracy. Hence, it is clear that the variation across the experiments is not explained by differences in either the achieved or potentially achievable accuracy.

Figure 5: Results using the the pseudo-maximum test set accuracy. Compare to Fig. 4.