In-N-Out: Pre-Training and Self-Training using Auxiliary Information for Out-of-Distribution Robustness

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Abstract

Consider a prediction setting where a few inputs (e.g., satellite images) are expensively annotated with the prediction targets (e.g., crop types), and many inputs are cheaply annotated with auxiliary information (e.g., climate information). How should we best leverage this auxiliary information for the prediction task? Empirically across three image and time-series datasets, and theoretically in a multi-task linear regression setting, we show that (i) using auxiliary information as input features improves in-distribution error but can hurt out-of-distribution (OOD) error; while (ii) using auxiliary information as outputs of auxiliary tasks to pre-train a model improves OOD error. To get the best of both worlds, we introduce In-N-Out, which first trains a model with auxiliary inputs and uses it to pseudolabel all the in-distribution inputs, then pre-trains a model on OOD auxiliary outputs and fine-tunes this model with the pseudolabels (self-training). We show both theoretically and empirically that In-N-Out outperforms auxiliary inputs or outputs alone on both in-distribution and OOD error.

1 Introduction

When models are tested on distributions that are different from the training distribution, they typically suffer large drops in performance [44, 2, 22, 17, 3]. For example, in remote sensing, central problems include predicting poverty, crop type, and land cover from satellite imagery for downstream humanitarian, policy, and environmental applications [52, 21, 49, 40]. In some developing African countries, labels are scarce due to the lack of economic resources to deploy human workers to conduct expensive surveys [21]. To make accurate predictions in these countries, we must extrapolate to out-of-distribution (OOD) examples across different geographic terrains and political borders to create a globally applicable model.

While labels are scarce, auxiliary information (e.g., climate data in remote sensing) is often available for every input. In many applications, we additionally have access to a large amount of unlabeled data (e.g., global satellite imagery) along with their corresponding auxiliary information. How should auxiliary information be used in this setting? One way is the use them directly as auxiliary input features (aux-inputs); another is to treat them as prediction outputs for an auxiliary task (aux-outputs) in pre-training or multi-task learning. Which approach is better for in-distribution or OOD performance?

In remote sensing, satellite imagery is paired with aux-inputs to predict the desired output [49, 54]. Aux-inputs can provide more features to improve in-distribution performance, and one may hope that this can also improve OOD performance. Indeed, previous results on standard datasets [28, 53, 11] show that improved in-distribution accuracy correlates with improves OOD accuracy. However, in this paper we find that while aux-inputs often help in-distribution error, they can hurt OOD error.

Conversely, aux-output methods such as pre-training, transfer learning, and multi-task learning may improve OOD performance by changing the inductive bias of the model through auxiliary supervi-
Figure 1: A sketch of the In-N-Out algorithm which consists of three steps: 1) use auxiliary information as input (Aux-in) to achieve good in-distribution performance, 2) use auxiliary information as output targets in pretraining (Aux-out), improving OOD performance, 3) fine-tune the pretrained model from step 2 using the labeled data and in-distribution unlabeled data with pseudo-labels generated by the Aux-in model from step 1.

Figure 2: Graphical model for our theoretical setting: prediction task with input $x$, targets $y$, and auxiliary information $z$ that is related to targets $y$ through the latent variable $w$ and latent noise $u$.

Hendrycks et al. [17] show that pretraining on ImageNet can improve adversarial robustness, and Hendrycks et al. [18] show that auxiliary self-supervision tasks can improve robustness to synthetic corruptions.

To theoretically study how to best use auxiliary information, we extend a multi-task linear regression setting [13, 46] to allow for distribution shifts. We show an example where auxiliary information helps in-distribution error by providing useful features for predicting the target, but the relationship between the aux-inputs and the target can shift significantly OOD, worsening the OOD error. In contrast, we prove that the aux-outputs model improves robustness to arbitrary covariate shift compared to the baseline by first pre-training on unlabeled data to learn a lower-dimensional representation and then solving the target task in the lower-dimensional space.

Can we do better than using auxiliary information as inputs or outputs alone? We propose the In-N-Out algorithm to combine the benefits of auxiliary inputs and outputs (Figure 1). In-N-Out first uses an aux-inputs model, which has good in-distribution accuracy, to pseudolabel in-distribution unlabeled data. Then we use these pseudolabels for self-training, where a pretrained model (using aux-outputs) is fine-tuned on the larger training set with labeled and pseudolabeled data. We prove that In-N-Out, which combines self-training and pretraining, further improves both in-distribution and OOD error over just pretraining.

We show empirical results on CelebA and two remote sensing tasks (land cover and cropland prediction) that matches the theory. On all datasets, In-N-Out improves OOD accuracy and has competitive or better in-distribution accuracy (1-2% in-distribution, 2-3% OOD over baseline on remote sensing tasks) over aux-inputs or aux-outputs alone. Ablations of In-N-Out also show that In-N-Out achieves similar improvements over pre-training or self-training alone (up to 5% in-distribution, 1-2% OOD on remote sensing tasks), and that using OOD unlabeled examples is important for OOD improvements.

2 Setup

Let $x \in \mathbb{R}^d$ be the input (e.g., a satellite image), $y \in \mathbb{R}$ be the target (e.g., crop type), and $z \in \mathbb{R}^T$ be auxiliary information—typically low-dimensional semantically meaningful features (e.g., soil type).

Training data. Let $P_{\text{id}}$ and $P_{\text{ood}}$ denote the underlying distribution of $(x,y,z)$ triples in-distribution and out-of-distribution, respectively. The training data consists of (i) in-distribution labeled data $\{(x_i,y_i,z_i)\}_{i=1}^n \sim P_{\text{id}}$, (ii) in-distribution unlabeled data $\{(x_{id,i},z_{id,i})\}_{i=1}^m \sim P_{\text{id}}$, and (iii) out-of-distribution...
unlabeled data \( \{(x_{i}^{\text{ood}}, z_{i}^{\text{ood}})\}_{i=1}^{m_{2}} \sim P_{\text{ood}} \).

**Loss metrics.** Our goal is to learn a model from input and auxiliary information to the target, \( f : \mathbb{R}^{d} \times \mathbb{R}^{T} \rightarrow \mathbb{R} \). For a loss function \( \ell \), the in-distribution population risk of the model \( f \) is 
\[
R_{\text{id}}(f) = \mathbb{E}_{x,y,z \sim P_{\text{id}}}[ \ell(f(x,z),y)],
\]
and its OOD population risk is 
\[
R_{\text{ood}}(f) = \mathbb{E}_{x,y,z \sim P_{\text{ood}}}[ \ell(f(x,z),y)].
\]

### 2.1 Models

We consider three common ways to use the auxiliary information \( z \) to learn a model.

**Baseline.** The baseline minimizes the empirical risk on labeled data while ignoring the auxiliary information (accomplished by setting \( z \) to 0):
\[
\hat{f}_{\text{bs}} = \arg\min_{f} \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_{i},0),y_{i}).
\]  

**Aux-inputs.** The aux-inputs model minimizes the empirical risk on labeled data while using the auxiliary information as features:
\[
\hat{f}_{\text{in}} = \arg\min_{f} \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_{i},z_{i}),y_{i}).
\]

**Aux-outputs.** The aux-outputs model leverages the auxiliary information \( z \) by using them as the prediction targets of \( T \) auxiliary tasks, in hopes that there is a low-dimensional feature representation that is common to predicting both \( z \) and \( y \). Training the aux-outputs model consists of two steps:

In the **pre-training** step, we use all the unlabeled data to learn a shared feature representation. Let \( h : \mathbb{R}^{d} \rightarrow \mathbb{R}^{k} \) denote a feature map and \( g_{\text{out}}^{z} : \mathbb{R}^{k} \rightarrow \mathbb{R}^{T} \) denote a mapping from feature representation to the auxiliary outputs. Let \( \ell_{\text{aux}} \) denote the loss function for the auxiliary information. We define the empirical risk of \( h \) and \( g_{\text{out}}^{z} \) as:
\[
\hat{R}_{\text{pre}}(h,g_{\text{out}}^{z}) = \frac{1}{m_{1}+m_{2}} \left( \sum_{i=1}^{m_{1}} \ell_{\text{aux}}(g_{\text{out}}^{z}(h(x_{i}^{\text{id}})),z_{i}^{\text{id}}) + \sum_{i=1}^{m_{2}} \ell_{\text{aux}}(g_{\text{out}}^{z}(h(x_{i}^{\text{ood}})),z_{i}^{\text{ood}}) \right).
\]  

The estimate of the feature map is \( \hat{h}_{\text{out}} = \arg\min_{h} \min_{g_{\text{out}}^{z}} \hat{R}_{\text{pre}}(h,g_{\text{out}}^{z}) \).

In the **transfer** step, the model uses the pre-trained feature map \( \hat{h}_{\text{out}} \) and the labeled data to learn the mapping \( g_{\text{out}}^{y} : \mathbb{R}^{k} \rightarrow \mathbb{R} \) from feature representation to target \( y \). We define the transfer empirical risk as:
\[
\hat{R}_{\text{trans}}(\hat{h}_{\text{out}},g_{\text{out}}^{y}) = \frac{1}{n} \sum_{i=1}^{n} \ell(g_{\text{out}}^{y}(\hat{h}_{\text{out}}(x_{i})),y_{i})
\]  

The estimate of the target mapping is \( \hat{g}_{\text{out}}^{y} = \arg\min_{g_{\text{out}}^{y}} \hat{R}_{\text{trans}}(\hat{h}_{\text{out}},g_{\text{out}}^{y}) \). The final aux-outputs model is
\[
\hat{f}_{\text{out}}(x,z) = \hat{g}_{\text{out}}^{y}(\hat{h}_{\text{out}}(x)).
\]

Like the baseline model, the aux-outputs model ignores the auxiliary information for prediction.

### 3 Theoretical Analysis of Aux-inputs and Aux-outputs Models

We now analyze the baseline, aux-inputs, and aux-outputs models introduced in Section 2. Our setup extends a linear regression setting commonly used for analyzing multi-task problems [13, 46].
Setup. See Figure 2 for the graphical model. Let $w = B^*x \in \mathbb{R}^k$ be a low-dimensional latent feature ($k \leq d$) shared between auxiliary information $z$ and the target $y$. Let $u \in \mathbb{R}^m$ denote unobserved latent variables not captured in $x$. We assume $z$ and $y$ are linear functions of $u$ and $w$:

$$y = \theta_w^T w + \theta_u^T u + \epsilon,$$

$$z = A^*w + C^*u,$$  \hspace{1cm} (6), (7)

where $\epsilon \sim P_{\epsilon}$ denotes noise with mean 0 and variance $\sigma^2$. As in [13], we assume $T \geq k$ and $T \geq m$ and $A^*, B^*$ and $C^*$ have rank $k$.

Data. Let $P_x$ and $P_u$ denote the underlying distribution of $x$ and $u$ in-distribution, and let $P'_x$, $P'_u$ denote their underlying distribution OOD. We assume $x$ and $u$ are independent, have bounded density everywhere, and have finite invertible covariance matrices. We assume the mean of $u$ is zero in- and out-of-distribution. We assume we have $n \geq m + d$ in-distribution labeled training examples and unlimited access to unlabeled data both in- and out-of-distribution, a common assumption in unsupervised adaptation [13] [27] [35].

Loss metrics. We use squared-error for target and auxiliary losses: $\ell(y, y) = (y - \hat{y})^2$ and $\ell_{aux}(z, z') = \|z - z'\|^2_2$.

Models. We assume all model families ($f$, $h$, $g_{out}^*$, $g_{out}^\star$) in Section 2 are linear.

Let $P = (A^*, B^*, C^*, \theta_w, \theta_u, P_x, P_u)$ denote the problem setting which satisfies all the assumptions.

3.1 Auxiliary inputs help in-distribution, but can hurt OOD

We show that the aux-inputs model (2) performs better than the baseline model (1) in-distribution but might perform worse than the baseline model OOD. Intuitively, the target $y$ depends on both the inputs $x$ (through $w$) and latent variable $u$ (Figure 2). The baseline model only uses $x$ to predict $y$; thus it cannot capture the variation in $y$ due to $u$. On the other hand, the aux-inputs model uses $x$ and $z$ to predict $y$. Since $z$ is a function of $x$ (through $w$) and $u$, $u$ can be recovered from $x$ and $z$ by inverting this relation. The aux-inputs model can then combine $u$ and $x$ to predict $y$ better.

Let $\sigma_u^2 = \mathbb{E}_{u \sim P_u}[(\theta_u^T u)^2]$ denote the (in-distribution) variance of $y$ due to the latent variables $u$. The following proposition shows that if $\sigma_u^2 > 0$ then with enough training examples the aux-inputs model has lower in-distribution population risk than the baseline model.

Proposition 1. For all problem settings $P$, $P_\epsilon$, assuming regularity conditions (bounded $x, u$, sub-Gaussian noise $\epsilon$, and $T = m$), and $\sigma_u^2 > 0$, for all $\delta > 0$, there exists $N$ such that for $n \geq N$ number of training points, with probability at least $1 - \delta$ over the training examples, the aux-inputs model improves over the baseline:

$$R_{id}(\hat{f}_{in}) < R_{id}(\hat{f}_{bs})$$  \hspace{1cm} (8)

Although using $z$ as input leads to better in-distribution performance, we show that the aux-inputs model can perform worse than the baseline model in OOD for any number of training examples. The aux-inputs model learns to predict $\hat{y} = \hat{\theta}^\top_{z, in} x + \hat{\theta}_{z, in} z$, where $\hat{\theta}_{z, in}$ is an approximation to the true parameter $\theta_z$, that has some error. Out-of-distribution $u$ and hence $z$ might have much higher variance than $x$, which would magnify the error $\hat{\theta}_{z, in} - \theta_z$ and lead to worse predictions.

Example 1. There exists a problem setting $P$, $P_\epsilon$, such that for every $n$, there is some test distribution $P'_x, P'_u$ with:

$$\mathbb{E}[R_{ood}(\hat{f}_{in})] > \mathbb{E}[R_{ood}(\hat{f}_{bs})]$$  \hspace{1cm} (9)

1This is not limiting because bias in $z$ can be folded into $x$.

2Since $z$ is typically low-dimensional and $x$ is high-dimensional (e.g. images), we only need a slightly larger number of examples for the aux-inputs model before it outperforms the baseline.
3.2 Pre-training improves risk under arbitrary covariate shift

While using \( z \) as inputs can worsen performance relative to the baseline, our first main result is that the aux-outputs model outperforms the baseline model under arbitrary covariate shifts.

**Theorem 1.** For all problem settings \( \mathcal{P}, P, \) and for all test distributions \( P^*_x \) and \( P^*_u \):

\[
\mathbb{E}[R_{ood}(f_{out})] \leq \mathbb{E}[R_{ood}(f_{bs})]
\]

See Appendix A for full proof. Intuitively, pre-training by learning a low rank linear model from \( x \) to \( z \) allows us to learn the lower dimensional feature space \( w = B^*x \) (up to symmetries). The aux-outputs model learns a linear map from the lower-dimensional \( w \) to \( y \), while the baseline predicts \( y \) directly from \( x \). Without distribution shift, standard techniques show that the aux-outputs model has better risk since \( w \) is lower dimensional than \( x \). In particular, the in-domain risk only depends on the dimension but not on the conditioning of the data. In contrast, the worst case risk under distribution shift depends on the conditioning of the data, which could be worse for \( w \) than \( x \). Our proof shows that the worst case risk (over all \( x \) and \( u \)) is still better for the aux-outputs model by “zeroing-out” error directions when projecting to the low-dimensional feature representation.

4 In-N-Out: combining auxiliary inputs and outputs

We propose the In-N-Out algorithm, which combines both the aux-inputs and aux-outputs models for further complementary gains (Figure 1). Since the aux-inputs model has better in-distribution performance, we use it to pseudolabel in-distribution unlabeled data (e.g. data from non-African locations). The pseudolabeled data provides more effective training samples (self-training) to fine-tune an aux-outputs model pre-trained on predicting auxiliary information from all unlabeled data (e.g. including Africa). We present the general In-N-Out algorithm in Algorithm 1 and then analyze it in the linear multi-task regression setting of Section 3. The In-N-Out model \( f = \hat{g} \circ \hat{h}_{out} \) optimizes the empirical risk on labeled and pseudolabeled data:

\[
\hat{g} = \arg \min_g (1 - \lambda) \hat{R}_{trans}(\hat{h}_{out}, g) + \lambda \hat{R}_{st}(g)
\]

where \( \hat{R}_{trans}(g) = \frac{1}{m} \sum_{i=1}^m \ell(\hat{g}(\hat{h}_{out}(x_i)), y_i) \) is the self-training loss on pseudolabels from the aux-inputs model, and \( \lambda \in [0, 1] \) is a hyperparameter that trades off between labeled and pseudolabeled losses. In our experiments, we fine-tune \( \hat{g} \) and \( \hat{h}_{out} \) together.

4.1 In-N-Out improves risk under arbitrary covariate shift

**Setup.** For the theory we analyze a slightly modified version of In-N-Out where the aux-inputs model is trained on the features \( \hat{h}_{out}(x) \) and we self-train on population unlabeled data. We train an aux-inputs model \( \hat{g}_{in} : \mathbb{R}^k \times \mathbb{R}^T \to \mathbb{R} \) given by \( \hat{g}_{in} = \arg \min_g \frac{1}{n} \sum_{i=1}^n \ell(g(\hat{h}_{out}(x_i), z_i), y_i) \). The self-training loss is:

\[
R_{st}(g) = \frac{1}{n} \sum_{i=1}^n \mathbb{E}_{z \sim P_z(x)} [\ell(g(\hat{h}_{out}(x_i), \hat{g}_{in}(\hat{h}_{out}(x_i), z_i)), y_i)]
\]

and we learn \( \hat{g} = \arg \min_g R_{st}(g) \). For input \( x, z \) the model outputs \( \hat{g}(\hat{h}_{out}(x)) \). For the theory, we assume all model families are linear.

We show that In-N-Out helps on top of pre-training, as long as the auxiliary features give us lots of information about \( y \) relative to the noise \( \epsilon \) in-distribution—in particular, if \( \sigma_u^2 \) is much larger than \( \sigma^2 \).
Theorem 2. In the linear setting, for all problem settings $P$ with $\sigma_u^2 > 0$, test distributions $P_{x', r_{x'}}, P_{x', r_{x'}}$, and $\delta > 0$, there exists $a, b > 0$ such that for all $P_x$, with probability at least $1 - \delta$ over the training examples and test example $x' \sim P_{x'}$, the ratio of the excess risks (for all $\sigma^2$ small enough that $a - b\sigma^2 > 0$) is:

\[
\frac{R_{ood} - R^*}{R_{out} - R^*} \leq \frac{\sigma^2}{a - b\sigma^2}
\]

Here $R^* = \min_{f^*} R_{ood}(f^*)$ is the minimum possible (Bayes-optimal) OOD risk, $R_{in-out} = \mathbb{E}_{y' \sim P_{y'|x'}} [\ell(g_{out}(y), y')]$ is the risk of the In-N-Out model on test example $x'$, and $R_{ood} = \mathbb{E}_{y' \sim P_{y'|x'}} [\ell(g_{ood}(y), y')]$ is the risk of the aux-outputs model on test example $x'$.

Remark 1. As $\sigma \rightarrow 0$, the excess risk ratio of In-N-Out to Aux-outputs goes to 0, and the In-N-Out estimator is much better than the aux-outputs estimator.

The proof of the result is in Appendix A, but we give high level intuition here. Since $u$ can be recovered from $w$ and $z$, we can write $y = \gamma_w w + \gamma_z z + \epsilon$. We train an aux-inputs model $g_{in}$ from $w, z$ to $y$ on finite labeled data—since the noise $\sigma^2 = \mathbb{E}[\epsilon^2]$ is small this model is very accurate. In the special case where $\epsilon = 0$, $g_{in}$ predicts $y$ perfectly from $w, z$. For each training example $w_i$, we sample many $z \sim P_z(x), w_i$, and pseudolabel the $w_i, z$ examples (very accurately). We then minimize the mean-squared error, which is equivalent to predicting the mean $\hat{y}_i$ of these pseudolabels from $w_i$. This essentially averages over latent noise $u$, so $\hat{y}_i$ is a denoised version of $\hat{y}_i$. In the special case where $\epsilon = 0$, the pseudolabel $\hat{y}_i = \theta_w w$ (without the u term) so we learn the Bayes-opt model $\theta_w$.

The technical challenge is proving that self-training helps under arbitrary covariate shift even when $\epsilon > 0$ (the aux-inputs model is very accurate but not perfect). The proof reduces to showing that the max singular value for the In-N-Out error matrix is less than the min-singular value of the aux-outputs error matrix with high probability. A core part of the argument is to lower bound the min-singular value of a random matrix (Lemma 3). This uses techniques from random matrix theory (see e.g. Chapter 2.7 in Tao [45]), the high level idea is to show that with probability $1 - \delta$ each column of the random matrix has a (not too small) component orthogonal to all other columns.

5 Experiments

We show on real-world remote sensing datasets for land cover prediction and cropland prediction that aux-inputs can hurt OOD performance, while aux-outputs improve OOD performance. In-N-Out improves OOD accuracy and has competitive or better in-distribution accuracy over other models on all datasets. Secondly, we show that the tradeoff between in-distribution and OOD performance depends on the choice of auxiliary information on CelebA and cropland prediction. Finally, we show that OOD unlabeled examples are important for improving OOD robustness.

5.1 Experimental Setup

We run experiments on the CelebA dataset [31] and two remote sensing datasets, Cropland and Landcover (see Figure 3 and Appendix B for details).

CelebA. In CelebA, the input $x$ is a RGB image (resized to $64 \times 64$), the target $y$ is a binary label for gender, and the auxiliary information $z$ are 7 (of 40) binary-valued attributes (e.g. presence of makeup, beard). We designate the set of images where the celebrity is wearing a hat as OOD. We use a ResNet18 as the backbone model architecture for all models (see Appendix B.1 for details).

Cropland. Crop type or cropland prediction is an important intermediate problem for crop yield prediction [5, 23, 28]. The input $x$ is a $50 \times 50$ RGB image taken by a satellite, the target $y$ is a binary label that is 1 when the image contains majority cropland, and the auxiliary information $z$ is the center location coordinate plus $50 \times 50$ vegetation-related bands. We use the Cropland dataset from Wang.
CelebA, Cropland, Landcover
Visualization (x) Aux Info (z) 7 binary attributes Vegetation, Lat/Lon Meteorological Data Target (y) Male/female? Cropland/not cropland? Land cover class ID-Split People without hats IA, MN, IL Outside Africa OOD-Split People with hats IN, KY Africa

Figure 3: Summary of the datasets used in our experiments.

CelebA Cropland Landcover
ID Test Acc OOD Acc ID Test Acc OOD Acc ID Test Acc OOD Test Acc
Baseline 90.46 ± 0.85 72.64 ± 1.39 94.50 ± 0.11 90.30 ± 0.75 75.92 ± 0.25 58.31 ± 1.87
Aux-inputs 92.36 ± 0.29 77.4 ± 1.33 95.34 ± 0.22 84.15 ± 4.23 76.58 ± 0.44 54.78 ± 2.01
Aux-outputs 94.0 ± 0.24 77.68 ± 0.59 95.12 ± 0.15 91.03 ± 0.21 72.48 ± 0.37 61.03 ± 0.97
In-N-Out (no pretrain) 93.8 ± 0.56 78.54 ± 1.31 94.93 ± 0.15 91.23 ± 0.61 76.54 ± 0.23 59.19 ± 0.98
In-N-Out 93.42 ± 0.36 79.42 ± 0.70 95.45 ± 0.16 91.94 ± 0.57 77.43 ± 0.39 61.53 ± 0.74
In-N-Out + repeated ST 93.76 ± 0.46 80.38 ± 0.68 95.53 ± 0.19 92.18 ± 0.40 77.10 ± 0.30 62.61 ± 0.58

Table 1: Accuracy (%) of various models using auxiliary information as input, output, or both. In-N-Out generally improves both in- and out-of-distribution over aux-inputs or aux-outputs alone. Results are averaged over 5 trials with 90% intervals. Repeated ST refers to one round of self-training on top of In-N-Out.

et al. [49], with data from the US Midwest. We designate Iowa, Missouri, and Illinois as in-distribution and Indiana and Kentucky as OOD. Following Wang et al. [49], we use a U-Net-based model [59]. See Appendix B.2 for details.

Landcover. Land cover prediction involves classifying the land cover type (e.g., “grasslands”) from satellite data at a location [15, 40]). The input $x$ is a time series measured by NASA’s MODIS satellite [48], the target $y$ is one of 6 land cover classes, and the auxiliary information $z$ is climate data (e.g. temperature) from ERA5, a dataset computed from various satellites and weather station data [4]. We designate non-African locations as in-distribution and Africa as OOD. We use a 1D-CNN to handle the temporal structure in the MODIS data. See Appendix B.3 for details.

Data splits. We first split off the OOD data, then randomly split the rest into training, validation, and in-distribution test (see Appendix B.3 for details). We use a portion of the training and OOD set as in-distribution and OOD unlabeled data respectively. The rest of the OOD set is held-out. We run 5 trials, where we regenerate the training/unlabeled split for each trial (keeping held-out splits fixed). We use a reduced number of labeled examples from each dataset (1%, 5%, 10% of labeled examples for CelebA, Cropland, and Landcover respectively), with the rest as unlabeled.

5.2 Main Results

Table 1 compares the in-distribution (ID) and OOD accuracy of different methods. Each method is trained with early-stopping and hyperparameters are chosen using the validation set. In our experiments, we also consider augmenting In-N-Out models with repeated self-training (repeated ST), which has fueled recent improvements in both domain adaptation and ImageNet classification [12, 53]. For one additional round of repeated ST, we use the In-N-Out model to pseudolabel all unlabeled data (both ID and OOD) and also initialize the weights with the In-N-Out model. In all datasets, pretraining with aux-outputs improves OOD performance over the baseline, and In-N-Out (with or without repeated
In-distribution accuracy

Figure 5: In-distribution vs. OOD accuracy when sequentially adding a random set of 15 auxiliary inputs one-by-one. While more auxiliary inputs generally improves both in-distribution and OOD accuracy, some in-distribution gains can hurt OOD.

Table 2: Ablation study on the use of in-distribution vs. OOD unlabeled data in pre-training models on Landcover, where unlabeled sample size is standardized (much smaller than Table 1). Using OOD unlabeled examples are important for gains in OOD accuracy (%). Results are shown with 90% error intervals over 5 trials.

|                | ID Test Acc | OOD Test Acc |
|----------------|-------------|--------------|
| Only in-distribution | 69.73 ± 0.51 | 57.73 ± 1.58 |
| Only OOD        | 69.92 ± 0.41 | 59.28 ± 1.01 |
| Both            | 70.07 ± 0.46 | 59.84 ± 0.98 |

CelebA. In CelebA, using auxiliary information either as aux-inputs or outputs improves both ID (2-4%) and OOD accuracy (5%). We hypothesize this is because the auxiliary information is quite robust. Figure 4 shows that there is a significant correlation ($r^2=0.52$) between ID and OOD accuracy for 100 different sets of aux-inputs, supporting results on standard datasets [38, 53, 41]. In-N-Out achieves the best OOD performance and comparable ID performance even though there is no tradeoff between ID and OOD accuracy.

Remote sensing. In our remote sensing datasets, aux-inputs can induce a tradeoff where increasing ID accuracy hurts OOD performance. In cropland prediction, even with a small geographic shift (US Midwest), the baseline model has a significant drop from ID to OOD accuracy (4%). The aux-inputs model improves ID accuracy almost 1% above the baseline but OOD accuracy drops 6%. In land cover prediction, using climate features as aux-inputs decreases OOD accuracy by over 4% compared to the baseline. The aux-outputs model improves OOD, but decreases ID accuracy by 3%. In both datasets, In-N-Out-based models generally improve both in- and OOD accuracy over all models.

Improving in-distribution accuracy over aux-outputs. One of the main goals of the self-training step in In-N-Out is to improve the in-distribution performance of the aux-outputs model. We compare to oracle models that use a large amount of in-distribution labeled data to compare the gains from In-N-Out. In Landcover, the oracle model which uses 150k labeled ID examples gets 80.5% accuracy. Since In-N-Out improves the ID accuracy of aux-output from 72.5% to 77.4%, we close most (62%) of the gap. In Cropland, the oracle model achieves 95.6% accuracy. Here, In-N-Out closes 80% of the gap between aux-outputs and the oracle, improving ID accuracy from 95.1% to 95.5%.

Ablations with only pretraining or self-training. We analyze the individual contributions of self-training and pretraining in In-N-Out. On both cropland and land cover prediction, In-N-Out outperforms standard self-training on pseudolabels from the aux-inputs model (In-N-Out without pretraining), especially on OOD performance, where In-N-Out improves by about 1% and 2% respectively. Similarly, In-N-Out improves upon pretraining (aux-outputs model) both ID and OOD for both datasets.

5.3 Choice of auxiliary inputs matters

We find that the choice of auxiliary inputs affects the tradeoff between ID and OOD performance significantly, and thus is important to consider for problems with distribution shift. While Figure 4 shows that auxiliary inputs tend to simultaneously improve ID and OOD accuracy in CelebA, our theory suggests that in the worst case, there should be auxiliary inputs that worsen OOD accuracy. Indeed, Figure 5 shows that when taking a random set of 15 auxiliary inputs and adding them sequentially as auxiliary inputs, there are instances where an extra auxiliary input improves in-distribution but hurts OOD accuracy. In cropland prediction, we compare using location coordinates and vegetation data as
auxiliary inputs with only using vegetation data. The model with locations achieves the best ID performance, improving almost 1% in-distribution over the baseline with only RGB. Without locations, the ID accuracy is similar to the baseline but the OOD accuracy improves by 1.5%. In this problem, location coordinates help with in-distribution interpolation, but the model fails to extrapolate on locations.

5.4 OOD unlabeled data is important for pretraining

We compare the role of in-distribution vs. OOD unlabeled data in pretraining. Table 2 shows the results of using only in-distribution vs. only OOD vs. a balanced mix of unlabeled examples for pretraining on the Landcover dataset, where unlabeled sample size is standardized across the models (by reducing to the size of the smallest set, resulting in 4x less unlabeled data). Using only in-distribution unlabeled examples does not improve OOD accuracy, while having only OOD unlabeled examples does well both in-distribution and OOD since it also has access to the labeled in-distribution data. For the same experiment in cropland prediction, the differences were not statistically significant, perhaps due to the smaller geographic shift (across states in cropland vs. continents in landcover).

6 Related work

Multi-task learning and weak supervision. Caruana and de Sa [8] proposed using poor input features as a multi-task output, but do not theoretically analyze this. Wu et al. [51] also study multi-task linear regression. However, their auxiliary tasks must have true parameters that are closely aligned (small cosine distance) to the target task. Similarly, weak supervision works assume access to weak labels correlated with the true label [37, 36]. In our paper, we make no assumptions about the alignment of the auxiliary and target tasks beyond a shared latent variable while also considering distribution shifts.

Transfer learning, pre-training, and self-supervision. We support empirical works that show the success of transfer learning and pre-training in vision and NLP [26, 24, 12]. Theoretically, Du et al. [13], Tripuraneni et al. [46] study pre-training in a similar linear regression setup. They show in-distribution generalization bound improvements, but do not consider OOD robustness or combining with auxiliary inputs. Hendrycks et al. [18] shows empirically that self-supervision can improve robustness to synthetic corruptions. We show similar robustness benefits for pre-training on auxiliary information (not part of the original input).

Self-training for robustness. [35] analyze robust self-training (RST) Carmon et al. [6], Najafi et al. [34], Usato et al. [47], which improves the tradeoff between standard and adversarially robust accuracy, in min-norm linear regression. While related, we work in multi-task linear regression, study pre-training, and prove robustness to arbitrary covariate shifts (rather than adversarial perturbations). Kumar et al. [27] show that repeated self-training on gradually shifting unlabeled data can enable adaptation over time. In-N-Out is complementary and may provide better pseudolabels in each step of this method. Chen et al. [9] show that self-training can remove spurious features for Gaussian input features in linear models, whereas our results hold for general input distributions (with density). Zoph et al. [55] show that self-training and pre-training combine for in-distribution gains. We provide theory to support this and also show benefits for OOD robustness.

Domain adaptation. Domain adaptation works account for covariate shift by using unlabeled data from a target domain to adapt the model [42, 19, 14]. Often, these methods [42, 19] have a self-training or entropy minimization component that benefits from having a better model in the target domain to begin with. Similarly, domain adversarial methods [14] rely on the inductive bias of the source-only model to correctly align the source and target distributions. In-N-Out may provide a better starting point for these domain adaptation methods.
7 Conclusion

We show that while auxiliary inputs improve in-distribution and OOD on standard curated datasets, they can hurt OOD in real-world datasets. In contrast, we show that using auxiliary information as outputs by pretraining improves OOD performance. In-N-Out combines the strengths of auxiliary inputs and outputs for further improvements. While a standard set of inputs and their auxiliary information may exist in many domains, the division between inputs and auxiliary information is not well-defined. Our framework applies generally to any division of the features, but an important further question is how to optimally choose what to use as auxiliary information under distribution shifts.

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A Proof for Sections 3 and 4

Our theoretical setting assumes all the model families are linear. We begin by specializing the setup in Section 2 and defining all the necessary matrices. A word on notation: if unspecified, expectations are taken over all random variables.

Data matrices: We have finite labeled data in-distribution: $n \geq d + m$ input examples $X \in \mathbb{R}^{n \times d}$, where each row $X_i \sim P_x$ is an example sampled independently. We have an unobserved latent matrix: $U \in \mathbb{R}^{n \times m}$ where each row $U_i \sim P_u$ is sampled independently from other rows and from $X$. $U$ is unobserved and not directly used by any of the models, but we will reference $U$ in our analysis. As stated in the main paper, we assume that $\mathbb{E}_{u \sim P_u}[u] = 0$. We have labels $Y \in \mathbb{R}^n$ and auxiliary data $Z \in \mathbb{R}^{n \times T}$, where each row $Y_i, Z_i$ is sampled jointly given input example $X_i, U_i$, that is: $Y_i, Z_i \sim P_{y,z|X_i, U_i}$. In our linear setting, we have $Z = X B^* \top A^* + U C^* \top$ and $Y = XB^* \top \theta_w + U \theta_u + \epsilon$, where $\epsilon \in \mathbb{R}^n$ with each entry $\epsilon_i \sim P_\epsilon$ sampled independently from a mean 0, variance $\sigma^2$ distribution $P_\epsilon$.

Reminder on shapes: As a reminder, $B^* \in \mathbb{R}^{k \times d}$ maps the input $x \in \mathbb{R}^d$ to a low dimensional representation $w \in \mathbb{R}^k$ via $w = B^* x$. $A^* \in \mathbb{R}^{T \times k}, C^* \in \mathbb{R}^{T \times m}$ generate auxiliary $z \in \mathbb{R}^T$ via: $z = A^* w + C^* u$. Finally, $y \in \mathbb{R}$ is given by: $y = \theta_w^\top w + \theta_u^\top u + \epsilon$, where $\theta_w \in \mathbb{R}^k, \theta_u \in \mathbb{R}^m$. Letting $\theta_z = B^* \top \theta_w$, we equivalently have $y = \theta_z^\top x + \theta_u^\top u + \epsilon$ in terms of $x, u$.

A.1 Models and Evaluation

Baseline: ordinary least squares estimator that uses $x$ only, so $\hat{\theta}_{x,\text{ols}} = \arg\min_{\theta'} \|Y - X \theta'\|_2$. Given a test example $x, z$, the baseline method predicts $\hat{f}_{\text{bs}}(x, z) = \hat{\theta}_{x,\text{ols}}^\top x$, ignoring $z$. In closed form, $\hat{\theta}_{x,\text{ols}} = (X^\top X)^{-1} X^\top Y$.

Aux-inputs: least squares estimator using $x$ and auxiliary $z$ as input: $\hat{\theta}_{x,\text{in}}, \hat{\theta}_{z,\text{in}} = \arg\min_{\theta', \theta''} \|Y - (X \theta' + Z \theta'')\|_2$. The input method predicts $\hat{\theta}_{x,\text{in}}^\top x + \hat{\theta}_{z,\text{in}}^\top z$ for a test example $x, z$. In closed form, letting $X_Z = [X; Z]$, we append the columns so that $X_Z \in \mathbb{R}^{n \times (d+T)}$, $\hat{\theta}_{x,\text{in}}, \hat{\theta}_{z,\text{in}} = (X_Z^\top X_Z)^{-1} X_Z^\top Y$.

Aux-outputs: pretrains on predicting $z$ from $x$ on unlabeled data to learn a mapping from $x$ to $w$, then learns a regression model on top of this latent embedding $w$. In the pretraining step: use unlabeled data to learn the feature-space embedding $B$:

$$\hat{A}, \hat{B} = \arg\min_{A, B} \mathbb{E}_{x \sim P_x} \|ABx - z\|_2^2 \quad A \in \mathbb{R}^{T \times k}, B \in \mathbb{R}^{k \times d}. \quad (13)$$
The transfer step solves a lower dimensional regression problem from $w$ to $y$: $\hat{\theta}_{w,\text{out}} = \arg\min_{\theta} \|Y - X\hat{B}^T\theta_{w}'\|_2$. Given a test example $x$, the output model predicts $\hat{\theta}_{w,\text{out}}^T\hat{B}x$.

**In-N-Out**: First learn an output model $\hat{A}, \hat{B}$, and let $W = X\hat{B}^T$ be the feature matrix. Next, train an input model on the feature space $w$. $\hat{\gamma}_{w,\text{out}} = \arg\min_{\gamma_{w,\text{out}}} \|Y - (W\gamma_{w} + Z\gamma_{z})\|_2$. Given a test example $x$, the output model predicts $\hat{\theta}_{w,\text{out}}^T\hat{B}x$.

Note that this is slightly different from our experiments where we trained the aux-inputs model directly on the inputs $x$. We now use the input model to pseudolabel our in-domain unlabeled examples, and self-train a model without $z$ on these pseudolabels. Given each point $w$, we produce a pseudolabel $E_z \sim P_{z\mid w}[\hat{\gamma}_w^T w + \hat{\gamma}_z^T z] = (\hat{\gamma}_w + A^T\hat{\gamma}_z)^T w$. We now learn a least squares estimator from $w$ to the pseudolabels which gives us the In-N-Out estimator $\hat{\theta}_w$:

$$\hat{\theta}_w = \hat{\gamma}_w + A^T\hat{\gamma}_z.$$ (15)

Note that we do not actually have access to $A$, this is just the closed form for the final estimator that self-training on the pseudolabels gives us. Given a test example $x$, In-N-Out predicts $\hat{\theta}_w^T\hat{B}x$.

### A.2 Auxiliary inputs help in-distribution

The proof of Proposition 1 is fairly standard. We first give a brief sketch, specify the additional regularity conditions, and then give the proof. We lower bound the risk of the baseline by $\sigma_u^2 + \sigma^2$ since this is the Bayes-opt risk of using only $x$ but not $z$ to predict $y$. We upper bound the risk of the aux-inputs model which uses $x, z$ to predict $y$, which is the same as upper bounding the risk in random design linear regression. For this upper bound we use Theorem 1 in Hsu et al. [20] (note that there are multiple versions of this paper, and we specifically use the Arxiv version, e.g. available at https://arxiv.org/abs/1106.2363). As such, we inherit their regularity conditions. In particular, we assume:

1. $x, u$ are upper bounded almost surely. This is a technical condition, and can be replaced with sub-Gaussian tail assumptions [20].
2. The noise $\epsilon$ is sub-Gaussian with variance parameter $\sigma^2$.
3. The latent dimension $m$ and auxiliary dimension $T$ are equal so that the inputs to the aux-inputs model have invertible covariance matrix.

**Restatement of Proposition 1** For all problem settings $\mathcal{P}, P_\epsilon$, assuming regularity conditions (bounded $x,u$, sub-Gaussian noise $\epsilon$, and $T = m$), and $\sigma_u^2 > 0$, for all $\delta > 0$, there exists $N$ such that for $n \geq N$ number of training points, with probability at least $1 - \delta$ over the training examples, the aux-inputs model improves over the baseline:

$$R_{id}(\hat{f}_m) < R_{id}(\hat{f}_{bs})$$ (16)

**Proof.** **Lower bound risk of baseline:** First, we lower bound the expected risk of the baseline by $\sigma_u^2 + \sigma^2$. Intuitively, this is the irreducible error—no linear classifier using only $x$ can get better risk than $\sigma_u^2 + \sigma^2$ because of intrinsic noise in the output $y$. Let $\theta_x = B^T\theta_w$ be the optimal baseline parameters.

---

Footnote: $x$ and $u$ are independent, with invertible covariance matrices, and $z = A^*B^*x + C^*u$ where $C^*$ is full rank, so by block Gaussian elimination we can see that $[x, z]$ has invertible covariance matrix as well.
We have

\[
R_{id}(\hat{f}_{b0}) = \mathbb{E}_{x,y,z \sim P_{id}} [(y - \hat{\theta}_{x,ols} x)^2]
\]  

(17)

\[
= \mathbb{E}_{x,u,\epsilon \sim P_{id}} [(\theta_x^T x + \theta_u^T u + \epsilon - \hat{\theta}_{x,ols} x)^2]
\]  

(18)

\[
= \mathbb{E}_{x \sim P_{id}} [(\theta_x^T x - \hat{\theta}_{x,ols} x)^2] + \mathbb{E}_{u \sim P_{id}} [\theta_u^T u^2] + \mathbb{E}_{\epsilon \sim P_{id}} [\epsilon^2]
\]  

(19)

\[
\geq \mathbb{E}_{u \sim P_{id}} [\theta_u^T u^2] + \mathbb{E}_{\epsilon \sim P_{id}} [\epsilon^2].
\]  

(20)

\[
= \sigma_u^2 + \sigma^2.
\]  

(21)

To get Equation (19), we expand the square, use linearity of expectation, and use the fact that \(x,u,\epsilon\) are independent where \(u,\epsilon\) are mean 0.

**Upper bound risk of aux-inputs:** On the other hand, we will show that if \(n\) is sufficiently large, the expected risk of the input model is less than \(\sigma_u^2 + \sigma^2\).

First we show that we can write \(y = \theta_x^T x + \theta_z^T z + \epsilon\) for some \(\theta_x, \theta_z\), that is \(y\) is a well-specified linear function of \(x\) and \(z\) plus some noise. Intuitively this is because \(y\) is a linear function of \(x,u\) and since \(C^*\) is invertible we can extract \(u\) from \(x,z\). Formally, we assumed the true model is linear, that is, \(y = \theta_x^T x + \theta_u^T u + \epsilon\). Since we have \(z = A^* B^* x + C^* u\) where \(C^*\) is invertible, we can write \(u = C^{-1}(z - A^* B^* x)\). This gives us

\[
y = \theta_x^T x + \theta_u^T u + \epsilon
\]  

(22)

\[
y = \theta_x^T x + \theta_u^T C^{-1}(z - A^* B^* x) + \epsilon
\]  

(23)

\[
y = (\theta_x - B^* A^* (C^* A^*)^{-1} \theta_u)^T x + (C^* A^*)^{-1} \theta_u^T z + \epsilon.
\]  

(24)

So setting \(\theta_x' = \theta_x - B^* A^* (C^* A^*)^{-1} \theta_u\) and \(\theta_z' = C^* A^*)^{-1} \theta_u\), we get \(y = \theta_x'^T x + \theta_z'^T z + \epsilon\).

As before, we note that the total mean squared error can be decomposed into the Bayes-opt error plus the excess error:

\[
R_{id}(\hat{f}_{aux}) = \mathbb{E}_{x,y,z \sim P_{id}} [(y - \hat{\theta}_{x,aux} x)^2]
\]  

(25)

\[
= \mathbb{E}_{x,z,\epsilon \sim P_{id}} [(\theta_x^T x + \theta_z^T z + \epsilon - \hat{\theta}_{x,aux} x - \hat{\theta}_{z,aux} z)^2]
\]  

(26)

\[
= \mathbb{E}_{x,z \sim P_{id}} [(\theta_x^T x + \theta_z^T z - \hat{\theta}_{x,aux} x - \hat{\theta}_{z,aux} z)^2] + \mathbb{E}_{\epsilon \sim P_{id}} [\epsilon^2]
\]  

(27)

\[
= \mathbb{E}_{x,z \sim P_{id}} [(\theta_x^T x + \theta_z^T z - \hat{\theta}_{x,aux} x - \hat{\theta}_{z,aux} z)^2] + \sigma^2.
\]  

(28)

To get Equation (27), we expand the square, use linearity of expectation, and use the fact that \(x,z,\epsilon\) are independent with \(\mathbb{E}[\epsilon] = 0\). So it suffices to bound the excess error, defined as:

\[
EE := \mathbb{E}_{x,z \sim P_{id}} [(\theta_x^T x + \theta_z^T z - \hat{\theta}_{x,aux} x - \hat{\theta}_{z,aux} z)^2]
\]  

(29)

To bound the excess error, we use Theorem 1 in Hsu et al. 20 where the inputs/covariates are \([x,z]\). \(\mathbb{E}[[x,z][x,z]^T]\) is invertible because \(m = T\), \(C^*\) is full rank, and \(P_x,P_u\) have density everywhere with density upper bounded so the variance in any direction is positive, and so the population covariance matrix is positive definite. This means \(\mathbb{E}[[x,z][x,z]^T]\) has min singular value lower bounded, and we also have that \(x, z\) are bounded random variables. Therefore, Condition 1 is satisfied for some finite \(\rho_0\). Condition 2 is satisfied since the noise \(\epsilon\) is sub-Gaussian with mean 0 and variance parameter \(\sigma^2\). Condition 3 is satisfied with \(b_0 = 0\), since we are working in the setting of well-specified linear regression.
To apply Theorem 1 [20], we first choose \( t = \log \frac{2}{\delta} \) so that \( 1 - 3e^{-t} \geq 1 - \delta \), and so the statement of the Theorem holds with probability at least \( 1 - \delta \). Since our true model is linear (or as Remark 9 says that “the linear model is correct”), \( \text{approx}(x) = 0 \).

So as per remark 9 [20] Equation 11, for some constant \( c' \), we have an upper bound on the excess error \( EE \) with probability at least \( 1 - \delta \):

\[
EE \leq \frac{\sigma^2(d + 2\sqrt{d}t + 2t)}{n} + o(1/n).
\]  

(30)

Note that the notation in Hsu et al. [20] is different. The learned estimator in ordinary least squares regression is denoted by \( \hat{\beta}_0 \), the ground truth parameters by \( \beta \), and the excess error is denoted by \( \| \hat{\beta}_0 - \beta \|_\Sigma \). See section 2.1, 2.2 of Hsu et al. [20] for more details.

Since \( t \) is fixed, there exists some constant \( c \) (dependent on \( \delta \)) such that for large enough \( N_1 \) if \( n \geq N_1 \):

\[
EE \leq \sigma^2(c/d/n).
\]  

(31)

Note that this is precisely Remark 10 [20]. Remark 10 says that \( \| \hat{\beta}_0 - \beta \|_\Sigma \) is within constant factors of \( \sigma^2 d/n \) for large enough \( n \). This is the variance term, but the bias term is 0 since the linear model is well-specified so \( \text{approx}(x) = 0 \). As in Propostion 2 [20] the total excess error is bounded by 2 times the sum of the bias and variance term, which gives us the same result.

Putting this (Equation 31) back into Equation 28 we get that with probability at least \( 1 - \delta \):

\[
R_{id}(\hat{f}_{in}) \leq \sigma^2(1 + cd/n).
\]  

(32)

Since \( \sigma_u^2 > 0 \), we have \( \sigma^2 < \sigma_u^2 + \sigma^2 \). Then for some \( N \) and for all \( n \geq N \), we have

\[
R_{id}(\hat{f}_{in}) < \sigma_u^2 + \sigma^2 \leq R_{id}(\hat{f}_{in}).
\]  

(33)

In particular, we can choose \( N = \max(N_1, c\sigma_u^2 d + 1) \), which completes the proof. \( \square \)

### A.3 Auxiliary inputs can hurt out-of-distribution

**Restatement of Example 1.** There exists a problem setting \( \mathcal{P}, P_x \), such that for every \( n \), there is some test distribution \( P_{x}, P_u \) with:

\[
\mathbb{E}[R_{ood}(\hat{f}_{in})] > \mathbb{E}[R_{ood}(\hat{f}_{bs})]
\]  

(34)

**Proof.** We will have \( x \in \mathbb{R} \) (so \( d = 1 \)), \( w = x \), and \( u, z \in \mathbb{R}^2 \). We set \( z_1 = u_1 + w \) and \( z_2 = u_2 \), in other words we choose \( A^* = [1, 0] \) and \( C^* = I_2 \) is the identity matrix. We set \( y = x + u_1 + \epsilon \), with \( \epsilon \sim N(0, \sigma^2) \), so \( y \) is a function of \( x \) and \( u_1 \) but not \( u_2 \). In other words we choose \( \theta_w = 1 \) and \( \theta_u = (1, 0) \). \( P_x \) will be Uniform\([-1, 1]\), and \( P_u \) will be uniform in the unit ball in \( \mathbb{R}^2 \).

Let \( X_Z = [X; Z] \), which denotes appending \( X \) and \( Z \) by columns so \( X_Z \in \mathbb{R}^{n \times 3} \) with \( n \geq 3 \). Since \( P_x \) and \( P_u \) have density, \( X_Z \) has rank 3 almost surely. This means that \( X_Z^\top X_Z \) is invertible (and positive semi-definite) almost surely. Since \( P_x \) and \( P_u \) are bounded, the maximum eigenvalue \( \tau_{max} \) of \( X_Z^\top X_Z \) is bounded above. The minimum eigenvalue \( \tau_{min} \) of \((X_Z^\top X_Z)^{-1}\) is precisely \( 1/\tau_{max} \) and is therefore positive and bounded below by some \( c > 0 \) almost surely.

We will define \( P' \) and \( P_u' \) soon. For now, consider a new test example \( x' \sim P'_{x}, u' \sim P_u' \) with \( z' = [x', 0] + u' \)
and $y' = x' + u'_1 + \epsilon'$ with $\epsilon' \sim N(0, \sigma')$ and $\mathbb{E}[u'] = 0$. For the input model we have:

$$
\mathbb{E}[R_{ood}(\hat{f}_{\text{in}})] = \mathbb{E}[\{y' - (\hat{\theta}_{x,\text{in}}^T x' + \hat{\theta}_{z,\text{in}}^T z')\}^2] \\
= \sigma^2 (1 + \mathbb{E}[(x', \hat{z})^T (X_z^T X_z)^{-1} (x', \hat{z})]) \\
\geq \sigma^2 (1 + \mathbb{E}[\sigma_{\min}^2 ((x', \hat{z})^T (\hat{z}))]) \\
\geq \sigma^2 (1 + c \mathbb{E}[(x', \hat{z})^T (\hat{z})]) \\
= \sigma^2 (1 + c \mathbb{E}[u'^2]) \\
= \sigma^2 (1 + c \mathbb{E}[u'^2]) \\
\geq \sigma^2 (1 + c \mathbb{E}[u'^2]) \quad (40)
$$

Notice that this lower bound is a function of $\mathbb{E}[u'^2]$ which we will make very large.

On the other hand, letting $\sigma_u^2 = \mathbb{E}_{u' \sim P_u'}[(\theta_u^T u')^2] = \mathbb{E}_{u' \sim P_u'}[u'^2]$, for the baseline model we have

$$
\mathbb{E}[R_{ood}(\hat{f}_{\text{bs}})] = \mathbb{E}[(y' - \hat{\theta}_x^T x')^2] \\
= \mathbb{E}[(\hat{\theta}_x^T x' + \hat{\theta}_x^T u' + \epsilon')^2] \\
= \mathbb{E}[(\hat{\theta}_x^T x' + \epsilon')^2 + \mathbb{E}[(\hat{\theta}_x^T x' + \hat{\theta}_x^T u')^2] \\
= \mathbb{E}[(\hat{\theta}_x^T x' + \epsilon')^2 + \mathbb{E}[(\hat{\theta}_x^T x')^2] + \mathbb{E}[(\hat{\theta}_x^T u')^2] \\
= \sigma_u^2 + \sigma^2 + \mathbb{E}[(\hat{\theta}_x^T x')^2] \\
= \sigma_u^2 + \sigma^2 + \mathbb{E}[x'^T (\hat{\theta}_x - \hat{\theta}_{x,\text{ols}})^T x'] \\
= \sigma_u^2 + \sigma^2 + \mathbb{E}[x'^T (\hat{\theta}_x - \hat{\theta}_{x,\text{ols}})^T x'] \\
\geq \sigma_u^2 + \sigma^2 + \mathbb{E}[x'^T (\hat{\theta}_x - \hat{\theta}_{x,\text{ols}})^T x'] \quad (47)
$$

where in Equation (46) we use the fact that $\theta_z - \hat{\theta}_{z,\text{ols}} = (X^T X)^{-1} X^T (U \theta + \epsilon)$ to get the next line. So the risk depends on $x'$ and $\mathbb{E}[u'^2]$ but not $\mathbb{E}[u'^2]$. So we choose $P_u' = \text{Uniform}(-1, 1)$. For $P_u'$, we sample the components independently, with $u'_1 \sim \text{Uniform}(-1, 1)$, and $u'_2 \sim \text{Uniform}(-R, R)$. By choosing $R$ large enough, we can make the lower bound for the input model arbitrarily large without impacting the risk of the baseline model which gives us

$$
\mathbb{E}[R_{ood}(\hat{f}_{\text{in}})] \geq \mathbb{E}[R_{ood}(\hat{f}_{\text{bs}})]. 
\quad (48)
$$

\[
\square
\]

### A.4 Pre-training improves risk under arbitrary covariate shift

**Restatement of Theorem 1.** For all problem settings $\mathcal{P}$, $P_e$, and for all test distributions $P'_y$ and $P'_u$:

$$
\mathbb{E}[R_{ood}(\hat{f}_{\text{out}})] \leq \mathbb{E}[R_{ood}(\hat{f}_{\text{bs}})] 
\quad (49)
$$

First we show that pre-training (training a low-rank linear map from $x$ to $z$) recovers the unobserved features $w$. We will then show that learning a regression map from $w$ to $y$ is better in all directions than learning a regression map from $x$ to $y$.

Our first lemma shows that we can recover the map from $x$ to $w$ up to identifiability (i.e., we will learn the rowspace of the true map from $x$ to $w$).

**Lemma 1.** For a pair $(x, z)$, let $z = A^* B^* x + \xi$ where $A^* \in \mathbb{R}^{T \times k}$ and $B^* \in \mathbb{R}^{k \times d}$ are the true parameters with $T, d \geq k$ and $\xi \in \mathbb{R}^T$ is mean-zero noise with bounded variance in each coordinate. Assume that $A^*, B^*$ are both rank $k$. Suppose that $\mathbb{E}[x x^T]$ is invertible. Let $\tilde{A}, \tilde{B}$ be minimizers of the population risk $\mathbb{E}[\|\tilde{A} \tilde{B} x - z\|^2]$ of the multiple-output regression problem. Then span${B^*_1, \ldots, B^*_k} = \text{span}{\tilde{B}_1, \ldots, \tilde{B}_k}$ where $B^*_i, \tilde{B}_i$ are the $i$-th rows of their respective matrices.
We show that the difference between the inner matrices is positive semi-definite, which implies the training targets are equal. Similarly the rowspace of $A$ and $B$ are equal. The rowspace of $A^*B^*$ is a subspace of the rowspace of $B^*$, but both have rank $k$ so they are equal. Similarly the rowspace of $\hat{A}B$ and $B$ are equal. This implies that the rowspace of $B$ and $B^*$ are equal, which is the desired result.

\[ \hat{A}B = A^*B^* \] (53)

By e.g. Sylvester’s rank inequality, $A^*B^*$ must be rank $k$, and so $\hat{A}B$ is rank $k$ (since they are equal). This means that $\hat{A},B$ are each rank $k$. Now $A^*B^*$ and $\hat{A}B$ have the same rowspace because they are equal. The rowspace of $A^*B^*$ is a subspace of the rowspace of $B^*$, but both have rank $k$ so they are equal. Similarly the rowspace of $\hat{A}B$ and $B$ are equal. This implies that the rowspace of $B$ and $B^*$ are equal, which is the desired result.

Our next lemma shows that for any fixed training examples $X$ and arbitrary test example $x'$, the aux-outputs model will have better expected risk than the baseline where the expectation is taken over the training labels $Y \mid X$.

**Lemma 2.** In the linear setting, fix data matrix $X$ and consider arbitrary test example $x'$. Let $\theta^* = B^\top \theta_w$ be the optimal (ground truth) linear map from $x$ to $y$. The expected excess risk of the aux-outputs model $\hat{B}^\top \hat{\theta}_{w,\text{out}}$ is better than for the baseline $\hat{\theta}_{x,\text{ols}}$, where the expectation is taken over the training targets $Y \sim P_{Y \mid X}$ ($Y$ shows up implicitly because the estimators $\hat{\theta}_{w,\text{out}}$ and $\hat{\theta}_{x,\text{ols}}$ depend on $Y$):

\[ \mathbb{E}[(\hat{\theta}_{w,\text{out}}^\top \hat{B}x' - \theta^* \top x')^2] \leq \mathbb{E}[(\hat{\theta}_{x,\text{ols}}^\top x' - \theta^* \top x')^2] \] (54)

**Proof.** Let $\epsilon_{\text{all}} = Y - X \theta^*$ be the training noise. From standard calculations, the instance-wise risk of $\hat{\theta}_{x,\text{ols}}$ for any $x$ is

\[ \mathbb{E}[(\hat{\theta}_{x,\text{ols}}^\top x' - \theta^* \top x')^2] = \mathbb{E}[(X^\top X)^{-1} X^\top Y \top x' - \theta^* \top x')^2] \] (55)

\[ = \mathbb{E}[(X^\top X)^{-1} X^\top \epsilon_{\text{all}} \top x' - \theta^* \top x')^2] \] (56)

\[ = \mathbb{E}[(X^\top X)^{-1} X^\top \epsilon_{\text{all}} \top x')^2] \] (57)

\[ = (\sigma^2 + \sigma_n^2) x'^\top (X^\top X)^{-1} x' \] (58)

By Lemma[1] $\hat{B} = QB$ for some full rank $Q$. Thus, learning $\hat{\theta}_{w,\text{out}}$ is a regression problem with independent mean-zero noise and we can apply the same calculations for the instance-wise risk of $\hat{B}^\top \hat{\theta}_{w,\text{out}}$.

\[ \mathbb{E}[(\hat{\theta}_{w,\text{out}}^\top \hat{B}x' - \theta^* \top x')^2] = (\sigma^2 + \sigma_n^2) x'^\top \hat{B}^\top (\hat{B}X^\top X \hat{B}^\top)^{-1} \hat{B} x'. \] (59)

We show that the difference between the inner matrices is positive semi-definite, which implies the result. In particular, we show that

\[ (X^\top X)^{-1} - \hat{B}^\top (\hat{B}X^\top X \hat{B}^\top)^{-1} \hat{B} \succeq 0. \] (60)
Since \( X^\top X \) is a full rank PSD matrix, we can write \( X^\top X = GG^\top \) for \( G \in \mathbb{R}^{d \times d} \) where \( G \) is full rank and therefore invertible. Expressing Equation [60] in terms of \( G \), we want to show:
\[
(GG^\top)^{-1} - \hat{B}^\top (\hat{B}GG^\top \hat{B}^\top)^{-1} \hat{B} \succ 0.
\] (61)

Left multiplying by \( G^\top \) and right multiplying by \( G \), which are both invertible, this is equivalent to showing:
\[
M := I - (\hat{B}G)^\top (\hat{B}GG^\top \hat{B}^\top)^{-1}(\hat{B}G) \succ 0.
\] (62)

But we note that \( M \) is symmetric, with \( M = M^2 = MM^\top \), so \( M \) is PSD. This completes the proof.

\[ \square \]

\textbf{Proof of Theorem 7} Fix training examples \( X \) and test example \( x' \) but let the train labels \( Y \sim P_{Y|X} \) and and test label \( y' \sim P_{y'|x'} \) be random. In particular, let \( \sigma_u^2 = \mathbb{E}[(\theta_u^\top u')^2] \) where \( u' \sim P_{u'} \), with \( \mathbb{E}[(u')^2] = 0 \). Then for the baseline OLS estimator, we have:
\[
\mathbb{E}[(y' - \hat{\theta}_{x,\text{ols}}' x')]^2 = \sigma_u^2 + \sigma^2 + \mathbb{E}[(\hat{\theta}_{x,\text{ols}}' x' - \theta x')^2] = \sigma_u^2 + \sigma^2 + \mathbb{E}[(\hat{\theta}_{x,\text{ols}}' x' - \theta x')^2] = \mathbb{E}[(y' - \hat{\theta}_{x,\text{ols}}' x')]^2
\] (63)

For the aux-outputs model, we have:
\[
\mathbb{E}[(y' - \hat{\theta}_{w,\text{out}}' \hat{B} x')]^2 = \sigma_u^2 + \sigma^2 + \mathbb{E}[(\hat{\theta}_{w,\text{out}}' \hat{B} x' - \theta x')^2] = \sigma_u^2 + \sigma^2 + \mathbb{E}[(\hat{\theta}_{w,\text{out}}' \hat{B} x' - \theta x')^2] = \mathbb{E}[(y' - \hat{\theta}_{w,\text{out}}' \hat{B} x')]^2
\] (64)

So applying Lemma 2, we get that the risk for the aux-outputs model is better than for the baseline (the lemma showed it for the excess risk):
\[
\mathbb{E}[(y' - \hat{\theta}_{w,\text{out}}' \hat{B} x')]^2 \leq \mathbb{E}[(y' - \hat{\theta}_{x,\text{ols}}' x')]^2
\] (65)

Since this is true for all \( X \) and \( x' \), it holds when we take the expectation over the training examples \( X \) from \( P_z \) and the test example \( x' \) from \( P_z^t \) which gives us the desired result.

\[ \square \]

\textbf{A.5 \text{In-N-Out} improves risk under arbitrary covariate shift}

\textbf{Restatement of Theorem 2} In the linear setting, for all problem settings \( \mathcal{P} \) with \( \sigma_a^2 > 0 \), test distributions \( P_{x',P_{u'}} \) and \( \delta > 0 \), there exists \( a, b > 0 \) such that for all \( P_z \), with probability at least \( 1 - \delta \) over the training examples and test example \( x' \sim P_{x'} \), the ratio of the excess risks (for all \( \sigma^2 \) small enough that \( a - b \sigma^2 > 0 \)) is:
\[
\frac{R_{\text{in-out}}^\text{ood}}{R_{\text{ood}}^*} \leq \frac{\sigma^2}{a - b \sigma^2}
\] (66)

Here \( R^{*} = \min f \cdot R_{\text{ood}}(f^*) \) is the minimum possible (Bayes-optimal) OOD risk, \( R_{\text{ood}} \) is the risk of the \text{In-N-Out} model on test example \( x' \), and \( R_{\text{ood}} = \mathbb{E}_{y' \sim P_{y'|x'}}[\ell(\hat{g}_{\text{ood}}(y'; x'), y')] \) is the risk of the aux-outputs model on test example \( x' \).

We first show a key lemma that lets us bound the min singular values of a random matrix, which will let us upper bound the risk of the \text{In-N-Out} estimator and lower bound the risk of the pre-training estimator.

\textbf{Definition 1.} As usual, the min singular value \( \tau_{\text{min}}(W) \) of a rectangular matrix \( W \in \mathbb{R}^{n \times k} \) where \( n \geq k \) refers to the k-th largest singular value (the remaining \( n-k \) singular values are all 0), or in other words:
\[
\tau_{\text{min}}(W) = \min_{\|\nu\|_2 = 1} \|W\nu\|_2.
\] (67)

\textbf{Lemma 3.} Let \( P_w \) and \( P_u \) be independent distributions on \( \mathbb{R}^k \) and \( \mathbb{R}^m \) respectively. Suppose they are absolutely continuous with respect to the standard Lebesgue measure on \( \mathbb{R}^k \) and \( \mathbb{R}^m \) respectively (e.g. this is true if they have density everywhere with density upper bounded). Let \( W \in \mathbb{R}^{n \times k} \) where each row \( W_i \) is sampled independently \( W_i \sim P_w \). Let \( U \in \mathbb{R}^{n \times m} \) where each row \( U_i \) is sampled independently \( U_i \sim P_u \). Suppose \( n \geq k + m \). For all \( \delta \), there exists \( c(\delta) > 0 \) such that with probability at least \( 1 - \delta \), the minimum singular values \( \tau_{\text{min}} \) are lower bounded by \( c(\delta) \cdot \tau_{\text{min}}(W) \), and \( \tau_{\text{min}}(\|W:U\|) > c(\delta) \).
Proof. We note that the matrices $W$ and $U$ are rectangular, e.g. $W \in \mathbb{R}^{n \times k}$ where $n \geq k$. We will prove the lemma for $W$ first, and the extension to $[W;U]$ will follow.

Note that removing the last $n-k$ rows of $W$ cannot increase its min singular value since that corresponds to projecting the vector $W \nu$ and projection never increases the Euclidean norm. So without loss of generality, we suppose $W$ only consists of its first $k$ rows and so $W \in \mathbb{R}^{k \times k}$.

Now, consider any row $W_i$. We will use a volume argument to show that with probability at least $1 - \frac{\delta}{k}$, this row $W_i$ has a non-trivial component perpendicular to all the other rows. Since all rows are independently and identically sampled, without loss of generality suppose $i = 1$. Fix the other rows $W_2, \ldots, W_k$, since $W_1$ is independent of these other rows, the conditional distribution of $W_1$ is the same as the marginal of $W_1$. The remaining rows $W_2, \ldots, W_k$ form a $k-1$ dimensional subspace $S$ in $\mathbb{R}^k$. Letting $d(w,S)$ denote the Euclidean distance of a vector $w$ from the subspace $S$, define the event $S_\lambda = \{ W_1 : d(W_1,S) \leq \lambda \}$. Since $P_w$ is absolutely continuous, $P(S_\lambda) \to 0$ as $\lambda \to 0$, so for some small $c(\delta) > 0$, $P(S_{c(\delta)}) < \frac{\delta}{k}$. So with probability at least $1 - \frac{\delta}{k}$, $d(W_1,S) > c(\delta)$.

By union bound, with probability at least $1 - \delta$, the distance from $W_i$ to the subspace spanned by all the other rows is greater than $c(\delta)$ for every row $W_i$, so we condition on this. By representing each row vector as the sum of the component perpendicular to $S$ and a component in $S$, applying Pythagoras theorem and expanding we get

$$\min_{\|\nu\|_2=1} \| W \nu \| = \min_{\|\nu\|_2=1} \|\nu^T W\| \geq c(\delta).$$

(68)

Which completes the proof for $\tau_{\min}(W)$.

For $[W;U]$, we note that $P_x$ and $P_u$ are independent, and the product measure is absolutely continuous. Since each row of $[W;U]$ is identically and independently sampled just like with $W$, we can apply the exact same argument as above (though for a different constant $c(\delta)$, we take the min of these two as our $c(\delta)$ in the lemma statement).

Recall that the In-N-Out estimator was obtained by fitting a model from $w,z$ to $y$, and then using that to produce pseudolabels on (infinite) unlabeled data, and then self-training a model from $w$ to $y$ on these pseudolabels. For the linear setting, we defined the In-N-Out estimator $\hat{\theta}_w$ in Equation 15. Our next lemma gives an alternate closed form of the In-N-Out estimator in terms of the representation matrix $W = X \hat{B}$ and the latent matrix $U$.

**Lemma 4.** In the linear setting, letting $W = X \hat{B}^\top$ we can write the In-N-Out estimator in closed form:

$$\hat{\theta}_w = [I_{k \times k};0_{k \times T}] \left( \begin{footnotesize} W^\top \end{footnotesize} \begin{footnotesize} U^\top \end{footnotesize} \right)^{-1} \begin{footnotesize} W^\top \end{footnotesize} Y.$$  

(69)

**Proof.** We recall the definition of the In-N-Out estimator, where we first train a classifier from $W, Z$ to $Y$:

$$\hat{\gamma}_{w,z} = \arg\min_{\gamma_{w,z}} \| Y - (W \gamma_w + Z \gamma_z) \|_2.$$  

(70)

Denote the minimum value of Equation 70 by $p^*$. Note that $\hat{\gamma}_{w,z}$ may not be unique, and we pick any solution to the argmin (although our proof will reveal that the resulting $\hat{\theta}_w$ is in fact unique). We then use this to produce pseudolabels and self-train, on infinite data, which gives us the In-N-Out estimator:

$$\hat{\theta}_w = \hat{\gamma}_w + A^\top \hat{\gamma}_z$$  

(71)

We will now consider the following alternative estimator:

$$\hat{\theta}'_w, \hat{\theta}'_u = \arg\min_{\hat{\theta}_w, \hat{\theta}_u} \| Y - (W \hat{\theta}'_w + U \hat{\theta}'_u) \|_2.$$  

(72)

Denote the minimum value of Equation 72 by $q^*$. We claim that $\hat{\theta}'_w = \hat{\theta}_w$. 

21
We have shown that the In-N-Out estimator $\hat{\theta}_w$ minimizes the alternative minimization problem in Equation [72] by showing that $p^* = q^*$. We will then show that the solution to Equation [72] is unique, which implies that $\theta'_w = \theta_w$.

We note that $C^{*\top} \in \mathbb{R}^{m \times T}$ where $T \geq m$ is full-rank, so there exists a right-inverse $C'$ with $C^{*\top} C' = I_{m \times m}$. Since $Z = WA^{*\top} + UC^{*\top}$, this gives us $U = (Z - WA^{*\top})C' = ZC' + W( -A^{*\top} C')$.

So this means that a solution to the alternative problem in Equation [72] can be converted into a solution for the original in Equation [70] with the same function value:

$$\min_{\theta'_w, \theta_u} \| Y - (W\hat{\theta}'_w + U\hat{\theta}_u) \|_2$$

$$= \min_{\theta'_w, \theta_u} \| Y - (W\hat{\theta}'_w + (ZC' + W( -A^{*\top} C'))\hat{\theta}_u) \|_2$$

$$= \min_{\theta'_w, \theta_u} \| Y - (W\hat{\theta}'_w - A^{*\top} C'\hat{\theta}_u + Z(C'\hat{\theta}_u)) \|_2.$$ (75)

This implies that $p^* \leq q^*$.

We now show that a solution to the original problem in Equation [70] can be converted into a solution for the alternative in Equation [72] with the same function value:

$$\min_{\gamma_w, \gamma_z} \| Y - (W\gamma_w + Z\gamma_z) \|_2$$

$$= \min_{\gamma_w, \gamma_z} \| Y - (W\gamma_w + (WA^{*\top} + UC^{*\top})\gamma_z) \|_2$$

$$= \min_{\gamma_w, \gamma_z} \| Y - (W(\gamma_w + A^{*\top} \gamma_z) + U(C^{*\top} \gamma_z)) \|_2.$$ (78)

This implies that $q^* \leq p^*$, and we showed before that $p^* \leq q^*$. But since $\gamma_w, \gamma_z$ minimizes the original minimizer in Equation [70] $\gamma_w + A^{*\top} \gamma_z, C^{*\top} \gamma_z$ minimize the alternative problem in Equation [72] where $\theta_w = \gamma_w + A^{*\top} \gamma_z$.

Since $[W:U]$ is full rank, the solution $\hat{\theta}'_w, \hat{\theta}_u$ to the alternative estimator Equation [72] is unique. So this means that $\theta'_w = \hat{\theta}_w$.

We have shown that $\hat{\theta}'_w = \hat{\theta}_w$—this completes the proof because solving Equation [72] for $\hat{\theta}_w$ gives us the closed form in Equation [69].

Next we show a technical lemma that says that if a random vector $u \in \mathbb{R}^n$ has bounded density everywhere, then for any $v$ with high probability the dot product $(u^\top v)^2$ cannot be too small relative to $\|v\|_2^2$.

**Lemma 5.** Suppose a random vector $u \in \mathbb{R}^n$ has density everywhere, with bounded density. For every $\delta$, there exists some $c(\delta)$ such that for all $v$, with probability at least $1 - \delta$ over $u$, $(u^\top v)^2 \geq c(\delta)\|v\|_2^2$.

**Proof.** First, we choose some $B_0$ such that $P(\|u\|_2 \geq B_0) \leq \delta/2$, such a $B_0$ exists for every probability measure.

Suppose that the density is upper bounded by $B_1$. Let the area of the $n-1$ dimensional sphere with radius $B_0$ be $A_0$. Consider any $n-1$ dimensional subspace $S$, and let $S_{\epsilon} = \{u' : d(u', S) \leq \epsilon\}$ where $d(u', S)$ denotes the Euclidean distance from $u'$ to $S$. We have $P(u \in S_{\epsilon}) \leq A_0 B_1 \epsilon + \delta/2$ for all $S_{\epsilon}$. By choosing sufficiently small $\epsilon > 0$, we can ensure that $P(u \in S) \leq \delta$ for all $S$.

Now consider arbitrary $v$ and let $S(v)$ be the $n-1$-dimensional subspace perpendicular to $v$. We have $P(u \in S(v)) \leq \delta$. But this means that $(u^\top v)^2 \geq \epsilon^2\|v\|_2^2$ with probability at least $1 - \delta$, which completes the proof.
By definition of our linear multi-task model, we recall that 
\[ y = \theta_w^T w + \theta_u^T u + \epsilon, \] 
where \( w = B^* x \). We do not have access to \( B^* \), but we assumed that \( B^* \) is full rank. We learned \( B \) which has the same rowspace as \( B^* \) (Lemma 1). This means that for some \( \theta'_w \), we have 
\[ y = \theta'_w^T \hat{w} + \theta_u^T u + \epsilon \] 
where \( \hat{w} = B x \). To simplify notation and avoid using \( \theta'_w \) and \( \hat{w} \) everywhere, we suppose without loss of generality that \( \hat{B} = B^* \) (but formally, we can just replace all the occurrences of \( \theta_w \) by \( \theta'_w \) and \( w \) by \( \hat{w} \)).

Our next lemma lower bounds the test error of the pre-training model.

**Lemma 6.** In the linear setting, for all problem settings \( P \) with \( \sigma_u^2 > 0 \), for all \( \delta \), there exists some \( a, b > 0 \) such that with probability at least \( 1 - \delta \) over the training examples and test example \( x' \sim P_x' \) the risk of the aux-outputs model is lower bounded:

\[ R^*_{\text{out}} - R^* > a - b \sigma^2. \]  

**Proof.** Recall that 
\[ R^*_{\text{out}} = \mathbb{E}_{y' \sim P_y'|x'}[l(\hat{f}_{\text{out}}(\hat{h}_{\text{out}}(x')), y')]. \]
Let \( \sigma_u'^2 = \mathbb{E}_{w' \sim P_w'}[(\theta_u^T w')^2] \). We have 
\[ R^* = \sigma^2 + \sigma_u'^2. \] 
Let \( W = X B^*^T \) be the feature matrix, where \( W \in \mathbb{R}^{n \times k} \).

Letting \( w' = B^* x' \), for the aux-outputs model we have

\[ \mathbb{E}_{y' \sim P_y'|x'}[(y' - \hat{\theta}_{w', out}^T w')^2] \]
\[ = \mathbb{E}_{y' \sim P_y'|x'}[(y' - \hat{\theta}_{w', out}^T w')^2] \]
\[ = (\sigma^2 + \sigma_u'^2) + (\theta_u^T w' - \hat{\theta}_{w', out}^T w')^2 \]
\[ = R^* + (\theta_u^T w' - \hat{\theta}_{w', out}^T w')^2. \]  

Let \( \epsilon = Y - (W \theta_w + U \theta_u) \) be the noise of \( Y \) for the training examples, which is a random vector with \( \epsilon \in \mathbb{R}^n \). We can now write

\[ (\theta_u^T w' - \hat{\theta}_{w', out}^T w')^2 = ((\epsilon + U \theta_u)^T W (W^T W)^{-1} w')^2. \]  

By assumption, \( W^T W \) is invertible (almost surely). With probability at least \( 1 - \delta/10 \) all entries of \( W^T W \) are upper bounded and we condition on this. So \( (W^T W)^{-1} \) has min singular value bounded below. By Lemma 3 \( W \) has min singular value that is bounded below with probability at least \( 1 - \delta/10 \). We condition on this being true. So let \( \nu = W(W^T W)^{-1} w' \), so for some \( c_0 > 0 \), we have \( ||\nu||_2 \geq c_0 ||w'||_2 \).

In terms of \( \nu \), we can write Equation 84 as

\[ (\theta_u^T w' - \hat{\theta}_{w', out}^T w')^2 = ((\epsilon + U \theta_u)^T \nu)^2 \]
\[ = (\epsilon^T \nu)^2 + ((U \theta_u)^T \nu)^2 + 2(\epsilon^T \nu)((U \theta_u)^T \nu) \]
\[ \geq ((U \theta_u)^T \nu)^2 + 2(\epsilon^T \nu)((U \theta_u)^T \nu) \]
\[ \geq ((U \theta_u)^T \nu)^2 - 2||\epsilon||_2 ||U \theta_u||_2 ||\nu||_2. \]  

We can find \( b_0 \) such that with at least probability \( 1 - \delta/10 \), \( ||(U \theta_u)^T\nu||_2 \leq b_0 \), condition on this. We note that \( \epsilon^T \nu \) has variance \( \sigma_u'^2 ||\nu||_2 \) so by Chebyshev for some \( b_1 \) with probability at least \( 1 - \delta/10 \), \( |\epsilon^T \nu| \leq b_1 \sigma_u^2 ||\nu||_2 \), condition on this. So we can now bound Equation 88 and get:

\[ (\theta_u^T w' - \hat{\theta}_{w', out}^T w')^2 \geq ((U \theta_u)^T \nu)^2 - 2b_0 b_1 \sigma_u^2 ||\nu||^2_2 \]  

Now we apply Lemma 3 where we use the fact that \( \sigma_u^2 > 0 \). So given \( \delta/10 \), there exists some \( c_1 \) such that for every \( \nu \) with probability at least \( 1 - \delta/10 \), \( ((U \theta_u)^T \nu)^2 \geq c_1 ||\nu||^2_2 \), giving us

\[ (\theta_u^T w' - \hat{\theta}_{w', out}^T w')^2 \geq (c_1 - 2b_0 b_1 \sigma_u^2) ||\nu||^2_2. \]
Since $w'$ has bounded density everywhere, it is non-atomic and we get that there is some $c_2 > 0$ such that with probability at least $1 - \delta/10$, $\|w'\|_2^2 \geq c_2^2$. But then $\|w\|_2^2 \geq c_0 c_2$, which gives us for some $a,b$, \[
abla \left( w \theta_w^T - \tilde{\theta}_w^T \right) w)^T = (c_1 - 2b_0 b_1 \sigma^2) c_0 c_2 \geq a - b \sigma^2. \] Combining this with Equation (93), we get with probability at least $1 - \delta$, \[
abla E_{y' \sim P_{y' \mid x'}} \left[ \left( \hat{f}_{\text{out}}(\tilde{h}_{\text{out}}(x')), y' \right) - R^* > a - b \sigma^2, \right. \] as desired.

\[\textbf{Lemma 7.} \text{ In the linear setting, for all problem settings } \mathcal{P}, \text{ for all } \delta, \text{ there exists some } c > 0 \text{ such that with probability at least } 1 - \delta \text{ over the training examples and test example } x' \sim P_x, \text{ the risk of the In-N-Out model is upper bounded:} \]
\[
R_{\text{ood}} - R^* < c^2. \]

\[\textbf{Proof.} \text{ Recall that } R_{\text{ood}} = \mathbb{E}_{y' \sim P_{y' \mid x'}} \left[ \left( \hat{f}_{\text{out}}(\tilde{h}_{\text{out}}(x')), y' \right) - R^* \right. \]
\[
\left. \left. - (\theta_w^T w' - \tilde{\theta}_w^T w') \right. \right]. \]

Now, taking the expectation over $W$, which is a random vector with bounded density everywhere, it is non-atomic and we get that there is some $c_2 > 0$ such that with probability at least $1 - \delta/10$, $\|w'\|_2^2 \geq c_2^2$. But then $\|w\|_2^2 \geq c_0 c_2$, which gives us for some $a,b$, \[
abla \left( w \theta_w^T - \tilde{\theta}_w^T \right) w)^T = (c_1 - 2b_0 b_1 \sigma^2) c_0 c_2 \geq a - b \sigma^2. \] Combining this with Equation (93), we get with probability at least $1 - \delta$, \[
abla E_{y' \sim P_{y' \mid x'}} \left[ \left( \hat{f}_{\text{out}}(\tilde{h}_{\text{out}}(x')), y' \right) - R^* > a - b \sigma^2, \right. \] as desired.

\[\textbf{Theorem 2} \text{ simply combines Lemma 6 and Lemma 7.} \]

\[\textbf{Proof of Theorem 2} \text{ For some } a,b,c, \text{ with probability at least } 1 - \delta, \text{ we have for the aux-outputs model:} \]
\[
R_{\text{ood}} - R^* > a - b \sigma^2, \]

and for the In-N-Out model:
\[
R_{\text{ood}} - R^* < c^2. \]

Taking ratios and dividing by suitable constants we get the desired result.
B Experimental details

B.1 CelebA

For the results in Table 1, we used 7 auxiliary binary attributes included in the CelebA dataset: ['Bald', 'Bangs', 'Mustache', 'Smiling', '5_o_Clock_Shadow', 'Oval_Face', 'Heavy_Makeup']. These attributes tend to be fairly robust to our distribution shift (not hat vs. hat) — if the person has a 5 o’clock shadow, the person is likely a man. We use a subset of the CelebA dataset with 2000 labeled examples, 30k in-distribution unlabeled examples, 3000 OOD unlabeled examples, and 1000 validation, in-distribution test, and OOD test examples each. The backbone for all models is a ResNet-18 [16] which takes a CelebA image downsized to $64 \times 64$ and outputs a binary gender prediction. All models are trained for 25 epochs using SGD with cosine learning rate decay, initial learning rate 0.1, and early stopped with an in-distribution validation set. The gender ratios in the in-distribution and OOD set are balanced to 50-50.

Aux-inputs model. We incorporate the auxiliary inputs by first training a baseline model $\hat{f}_{bs}$ from images to output logit, then training a logistic regression model on the concatenated features $[\hat{f}_{bs}(x); z]$ where $z$ are the auxiliary inputs. We sweep over L2 regularization hyperparameters $C = \{0.1, 0.5, 1.0, 5.0, 10.0, 20.0, 50.0\}$ and choose the best with respect to an in-distribution validation set.

Aux-outputs model. During pretraining, the model trains on the 7-way binary classification task of predicting the auxiliary information. Then, the model is finetuned on the gender classification task without auxiliary information.

In-N-Out and repeated self-training. For In-N-Out models with repeated self-training, we pseudolabeled all the unlabeled data using the In-N-Out model and did one round of additional self-training. Following [27], we employ additional regularization when doing self training by adding dropout with probability 0.8. We also reduced the learning rate to 0.05 to improve the training dynamics.

Adding auxiliary inputs one-by-one. In Figure 5, we generate a random sequence of 15 auxiliary inputs and add them one-by-one to the model, retraining with every new configuration. We use the following auxiliary information: 'Young', 'Straight_Hair', 'Narrow_Eyes', 'Mouth_Slightly_Open', 'Blond_Hair', '5_o_Clock_Shadow', 'Big_Nose', 'Oval_Face', 'Chubby', 'Attractive', 'Blurry', 'Goatee', 'Heavy_Makeup', 'Wearing_Necklace', and 'Bushy_Eyebrows'.

Correlation between in-distribution and OOD accuracy. In Figure 4, we sample 100 random sets of auxiliary inputs of sizes 1 to 15 and train 100 different aux-inputs models using these auxiliary inputs. We plot the in-distribution and OOD accuracy for each model, showing that there is a significant correlation between in-distribution and OOD accuracy in CelebA, supporting results on standard datasets [38, 53, 41]. Each point in the plot is an averaged result over 5 trials.

B.2 Cropland

All models reported in Table 1 were trained using the Adam optimizer with learning rate 0.001, a batch size of 256, and 100 epochs unless otherwise specified. Our dataset consists of about 7k labeled examples, 170k unlabeled examples (with 130k in-distribution examples), 7.5k examples each for validation and in-distribution test, and 4260 OOD test examples (the specification of OOD points is described in further detail below). Results are reported over 5 trials, and $\lambda \in \{0.5, 0.6, 0.7, 0.8, 0.9\}$ was chosen using the validation set.

Problem Motivation. Developing machine learning models trained on remote sensing data is currently a popular line of work for practical problems such as typhoon rainfall estimation, monitoring reservoir water quality, and soil moisture estimation [20, 33, 41]. Models that could use remote sensing
data to accurately forecast crop yields or estimate the density of regions dedicated to growing crops would be invaluable in important tasks like estimating a developing nation’s food security [20].

**OOD Split.** In remote sensing problems it is often the case that certain regions lack labeled data (e.g., due to a lack of human power to gather the labels on site), so extrapolation to these unlabeled regions is necessary. To simulate this data regime, we use the provided (lat, lon) pairs of each data point to split the dataset into labeled (in-distribution) and unlabeled (out-of-distribution) portions. Specifically, we take all points lying in Iowa, Missouri, and Illinois as our ID points and use all points within Indiana and Kentucky as our OOD set.

**Shape of auxiliary info.** To account for the discrepancy in shapes of the two sources of auxiliary information (latitude and longitude are two scalar measurements while the 3 vegetation bands form a $3 \times 50 \times 50$ tensor), we create latitude and longitude “bands” consisting of two $50 \times 50$ matrices that repeat the latitude and longitude measurement, respectively. Concatenating the vegetation bands and these two pseudo-bands together gives us an overall auxiliary dimension of $5 \times 50 \times 50$.

**UNet.** Since our auxiliary information takes the form of $50 \times 50$ bands, we need a model architecture that can reconstruct these bands in order to implement the aux-outputs and the In-N-Out models. With this in mind, we utilize a similar UNet architecture that Wang et al. [19] use on the same Cropland dataset. While the UNet was originally proposed by Ronneberger et al. [39] for image segmentation, it can be easily modified to perform image-to-image translation. In particular, we remove the final $1 \times 1$ convolutional layer and sigmoid activation that was intended for binary segmentation and replace them with a single convolutional layer whose output dimension matches that of the auxiliary information. In our case, the last convolutional layer has an output dimension of 5 to reconstruct the 3 vegetation bands and (lat, lon) coordinates.

To perform image-level binary classification with the UNet, we also replace the final $1 \times 1$ convolutional layer and sigmoid activation, this time with a global average pool and a single linear layer with an output dimension of 1. During training we apply a sigmoid activation to this linear layer’s output to produce a binary class probability, which is then fed into the binary cross entropy loss function.

**Aux-inputs model.** Since the original RGB input image is $3 \times 50 \times 50$, we can simply concatenate the auxiliary info alongside the original image to produce an input of dimensions $8 \times 50 \times 50$ to feed into the UNet.

**Aux-outputs model.** The modification of the traditional UNet architecture in order to support auxiliary outputs for Cropland is described in the above UNet section. We additional add a tanh activation function to squeeze the model’s output values to the range $[-1, 1]$ (the same range as the images). We train the model to learn the auxiliary bands via pixel-wise regression using the mean squared error loss.

**In-N-Out model.** We found that the finetuning phase of the In-N-Out algorithm experienced wild fluctuations in loss and would not converge when using the hyperparameters listed at the top of this section. To encourage the model to converge and fit the training set, we decreased the Adam learning rate to 0.0001 and doubled the batch size to 512.

**Repeated self-training.** For the additional round of self-training, we initialize training and pseudolabel all unlabeled data with the In-N-Out model. Following [27], we employ additional regularization when doing self-training by adding dropout with probability 0.8.

**B.3 Landcover**

Our Landcover dataset comes from NASA’s MODIS Surface Reflectance product, which is made up of measurements from around the globe taken by the Terra satellite [48]. In each trial, we use about 16k labeled examples from non-African locations, 203k unlabeled examples (with 150k in-distribution
examples), 9266 examples each for validation and in-distribution test, and 4552 OOD test examples. We trained with SGD + momentum (0.9) on all models for 400 epochs with a cosine learning rate schedule. We used learning rate 0.1 for all models that were not pre-trained, and learning rate 0.01 for models that were already pre-trained. Results are reported over 5 trials, and $\lambda \in \{0.1, 0.3, 0.5, 0.7, 0.9\}$ was chosen using the validation set.

1D CNN While Convolutional Neural Networks are most commonly associated with the groundbreaking success of 2D-CNNs on image-based tasks, the 1-dimensional counterparts have also found success in various applications [23]. Because the measurements from the MODIS satellite are not images but instead scalar-valued time series data, we can use a 1D CNN with 7 channels, one for each of the 7 MODIS sensors.

NDVI The normalized difference vegetation index (NDVI) is a remote sensing measurement indicating the presence of live green vegetation. It has been shown to be a useful predictor in landcover-related tasks [11, 10, 32], so we choose to include it in our models as well. NDVI can be computed from the RED and NIR bands of the MODIS sensors via the equation

$$\text{NDVI} = (\text{NIR} - \text{RED}) / (\text{NIR} + \text{RED}).$$

We include NDVI along with the 7 other MODIS bands to give us input dimensions of $46 \times 8$.

ERA5 It is a reasonable hypothesis that having additional climate variables such as soil type or precipitation could be useful for a model in inferring the underlying landcover class. To this end we incorporate features from the ERA5 climate dataset as our auxiliary information [4]. The specific variables we include are soil type, temperature, precipitation rate, precipitation total, solar radiation, and cloud cover. For each MODIS point we find its nearest ERA5 neighbor based on their latitude and longitude in order to pair the datasets together.

The ERA5 measurements are monthly averages, which means the readings are at a different frequency than that of the 8-day MODIS time series. We upsample the ERA5 signal using the `scipy.signal.resample` method, which uses the FFT to convert to the frequency domain, adds extra zeros for upsampling to the desired frequency, and then transforms back into the time domain.

Landcover classes. The Landcover dataset has a total of 16 landcover classes, with a large variance in the individual class counts. To ensure our model sees enough examples of each class, we filtered the dataset to include just 6 of the most populous classes: savannas, woody_savannas, croplands, open_shrublands, evergreen_broadleaf_forests, and grasslands.

Aux-inputs model. We concatenate the resampled ERA5 readings with the MODIS and NDVI measurements to obtain an input dimension of $46 \times 14$.

Aux-outputs model. Rather than predicting the entire ERA5 time series as an auxiliary output, we instead average the 6 climate variables over the time dimension and predict those 6 means as the auxiliary outputs. We use a smaller learning rate of 0.01 for this pre-trained model.

In-N-Out and Repeated self-training. The In-N-Out model initializes its weights from the aux-outputs model and gets pseudolabeled ID unlabeled data from the aux-inputs model. As with aux-outputs, we use a smaller learning rate of 0.01 for this pre-training model.

For the additional round of self-training, we initialize training and pseudolabel all unlabeled data with the In-N-Out model. Following [27], we employ additional regularization when doing self training by adding dropout with probability 0.5. We found that with dropout, we need a higher learning rate (0.1) to effectively fit the training set.