Tailoring: encoding inductive biases by optimizing unsupervised objectives at prediction time

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Abstract

From CNNs to attention mechanisms, encoding inductive biases into neural networks has been a fruitful source of improvement in machine learning. Adding auxiliary losses to the main objective function is a general way of encoding biases that can help networks learn better representations. However, since auxiliary losses are minimized only on training data, they suffer from the same generalization gap as regular task losses. Moreover, by adding a term to the loss function, the model optimizes a different objective than the one we care about. In this work we address both problems: first, we take inspiration from *transductive learning* and note that after receiving an input but before making a prediction, we can fine-tune our networks on any unsupervised loss. We call this process *tailoring*, because we customize the model to each input to ensure our prediction satisfies the inductive bias. Second, we formulate *meta-tailoring*, a nested optimization similar to that in meta-learning, and train our models to perform well on the task objective after adapting them using an unsupervised loss. The advantages of tailoring and meta-tailoring are discussed theoretically and demonstrated empirically on a diverse set of examples.

1 Introduction

The key to successful generalization in machine learning is the encoding of useful inductive biases. A variety of mechanisms, from parameter tying to data augmentation, have proven useful to improve the performance of models. Among these, auxiliary losses can encode a wide variety of biases, constraints, and objectives; helping networks learn better representations and generalize more broadly. Auxiliary losses add an extra term to the task loss that is minimized over the training data.

However, they have two major problems:

1. Auxiliary losses are only minimized at training time, but not for the query points. This leads to a generalization gap between training and testing, in addition to that of the task loss.
2. By minimizing the sum of the task loss plus the auxiliary loss, we are optimizing a different objective than the one we care about (only the task loss).

In this work we propose a solution to each problem:

1. We use ideas from *transductive learning* to minimize unsupervised auxiliary losses at each query, thus eliminating their generalization gap. Because these losses are unsupervised, we can optimize them at any time inside the prediction function. We call this process *tailoring*, since we customize the model to each query.
2. We use ideas from *meta-learning* to learn a model that performs well on the task loss after being tailored with the unsupervised auxiliary loss. *Meta-tailoring* effectively trains the model to leverage the unsupervised tailoring loss in order to minimize the task loss.

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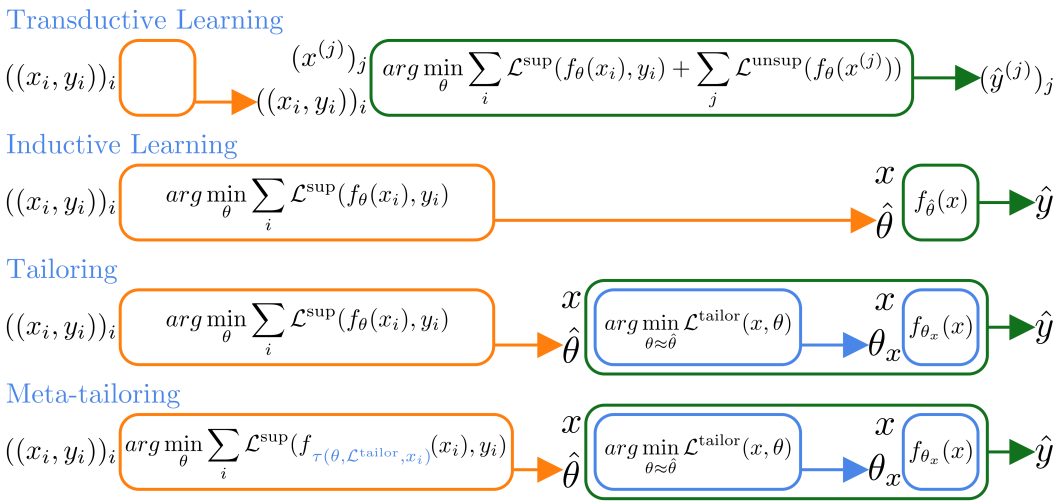

Figure 1: Comparison of several learning settings with *offline* computation in the orange boxes and *online* computation in the green boxes, with tailoring in blue. For meta-tailoring training, $\tau(\theta, \mathcal{L}^{\text{tailor}}, x) = \text{argmin}_{\theta' \approx \theta} \mathcal{L}^{\text{tailor}}(x, \theta')$ represents the tailoring process resulting in θ_x.

Tailoring a predictor Traditionally, supervised learning is approached within the inductive learning framework, shown in the second row of Figure 1. There, an algorithm consumes a training dataset of input-output pairs, $((x_i, y_i))_{i=1}^n$, and produces a set of parameters $\hat{\theta}$ by minimizing a supervised loss $\sum_{i=1}^n \mathcal{L}^{\text{sup}}(f_\theta(x_i), y_i)$ and, optionally, an unsupervised auxiliary loss $\sum_{i=1}^n \mathcal{L}^{\text{unsup}}(\theta, x_i)$. These parameters specify a hypothesis $f_{\hat{\theta}}(\cdot)$ that, given a new input x, generates an output $\hat{y} = f_{\hat{\theta}}(x)$. This problem setting misses a substantial opportunity: before the learning algorithm sees the query point x, it has distilled the data down to the parameters $\hat{\theta}$, which are frozen during inference, and so it cannot use new information about the *particular* x that it will be asked to make a prediction for.

Vapnik recognized an opportunity to make more accurate predictions when the query point is known, in a framework that is now known as *transductive learning* [48, 11], illustrated in the top row of Figure 1. In transductive learning, a single algorithm consumes both labeled data, $((x_i, y_i))_{i=1}^n$, and a set of input queries for which predictions are desired, $(x^{(j)})_j$, and produces predicted outputs $(\hat{y}^{(j)})_j$ for each query. In general, however, we do not know queries *a priori*, and instead, we want an inductive function that makes predictions online, as queries arrive. To obtain such an online prediction function from a transductive system, we would need to encapsulate the entire transductive learning procedure inside the prediction function itself. This strategy would achieve our objective of taking x into account at prediction time but would be computationally much too slow.

This approach for combining induction and transduction would reuse the same training data and objective for each prediction, only changing the single unlabeled query. Consequently, it would perform extremely similar computations for each prediction. Therefore, we propose to effectively reuse the shared computations and find a "meta-hypothesis" that can then be efficiently adapted to each query. As shown in the third row of Figure 1, we first run regular supervised learning to obtain parameters $\hat{\theta}$. Then, given a query input x, we fine-tune $\hat{\theta}$ on an unsupervised loss $\mathcal{L}^{\text{tailor}}$ to obtain customized parameters θ_x and use them to make the final prediction: $f_{\theta_x}(x)$. We call this process *tailoring*, because we adapt the model to each particular input for a customized fit. Notice that tailoring optimizes the loss at the query input, eliminating the generalization gap on the unsupervised auxiliary loss.

Meta-tailoring Since we will be applying tailoring at prediction time, it is natural to incorporate this adaptation during training, resulting in a two-layer optimization similar to those used in meta-learning. Because of this similarity, we call this process *meta-tailoring*, illustrated in the bottom row of Figure 1. Now, rather than letting $\hat{\theta}$ be the direct minimizer of the supervised loss, we set it to

$$\hat{\theta} \in \arg\min_\theta \sum_{i=1}^n \mathcal{L}^{\text{sup}}(f_{\tau(\theta, \mathcal{L}^{\text{tailor}}, x_i)}(x_i), y_i).$$

Here, the inner loop optimizes the unsupervised tailoring loss $\mathcal{L}^{\text{tailor}}$ and the outer loop optimizes the supervised task loss $\mathcal{L}^{\text{sup}}$. Notice that now the outer process optimizes the only objective we care, $\mathcal{L}^{\text{sup}}$, instead of a proxy combination of $\mathcal{L}^{\text{sup}}$ and $\mathcal{L}^{\text{unsup}}$. At the same time, we learn to leverage $\mathcal{L}^{\text{tailor}}$ in the inner loop to affect the model before making the final prediction, both during training and evaluation.

In many settings, we want to make predictions for a large number of queries in a (mini-)batch. While naively tailoring adapts to every input separately, we can ensure it can run in parallel efficiently. Inspired by conditional normalization (CN) [17] we propose CNGRAD, which adds element-wise affine transformations to our model and only adapts the added parameters in the inner loop. This allows us to independently *tailor* the model for multiple inputs in parallel. We prove theoretically, in Sec. 4, and provide experimental evidence, in Sec. 5.1, that optimizing these parameters alone has enough capacity to minimize a large class of tailoring losses.

Relation between (meta-)tailoring, fine-tuning transfer, and meta-learning Fine-tuning pre-trained networks is a fruitful method of transferring knowledge from large data corpora to smaller related datasets [16]. Fine-tuning allows reusing features on related but different tasks or for different distributions of the same task. When the data we want to adapt to is unlabeled, we must use unsupervised losses. This can be useful to adapt to changes of task [15], from simulated to real data [50], or changes in distribution [44].

Tailoring performs unsupervised fine-tuning and is, in this sense, similar to test-time training [44] for a single sample, which was developed for adapting to distribution shifts. However, tailoring is applied to a single query and not to a large data set that captures distribution shift, where batched test-time training sees most of its benefits. Thus, whereas fine-tuning always benefits from more adaptation data, tailoring is hindered by more data. This is because tailoring aims at building a custom model for each query to ensure the network satisfies a particular inductive bias. Customizing the model to multiple samples would make this goal harder, not easier. We show this in Figure 2, where test-time training with 6400 samples performs worse than tailoring with a single sample. Furthermore, tailoring adapts to each query one by one, not globally from training data to test data. Therefore, it also makes sense to do tailoring for training queries, which brings us to meta-tailoring.

Meta-tailoring has the same two-layer optimization structure as meta-learning. More concretely, it can be understood as the extreme case of meta-learning where each single-query prediction is its own task. However, whereas meta-learning tasks use one loss and different examples for the inner and outer loop, meta-tailoring tasks use different losses and one example for each loop ($\mathcal{L}^{\text{tailor}}$, $\mathcal{L}^{\text{sup}}$). We emphasize that meta-tailoring does not operate in the typical multi-task meta-learning setting. Instead, we are leveraging techniques from meta-learning for the classical single-task ML setting.

Losses for tailoring Tailoring can be used any time we are making a prediction and have an unsupervised loss that can be minimized on the current input. Many types of *tailoring* losses can be useful; here we enumerate three broad classes.

<u>Losses imposing priors and constraints satisfied by the correct predictions.</u> For instance, we can enforce conservation of momentum and energy when learning a physics model, symmetry under specific transformations, or cycle-consistency when learning to translate between two languages. We show that tailoring a loss of this type improves predictive losses in sections 5.1 and 5.2.

<u>Losses that help learn better representations,</u> such as the contrastive losses [23] explored in semi-supervised learning, or learning to predict one part of the input from another part, like depth from RGB [34]. In sections 3.1 and 5.3, we show theoretically and with experiments that tailoring with a contrastive loss improves supervised prediction performance. <u>Losses informed by theoretical guarantees.</u> The guarantees of many theorems depend on unsupervised quantities, such as smoothness or distance to the prediction boundary. By optimizing such quantities on the query, or the surrounding area, we can get better-guaranteed performance. In section 5.4, we show this on adversarial examples, where smooth predictions around the query point are critical.

Contributions In summary, our contributions are:

1. Introducing *tailoring*, a new framework for encoding inductive biases by minimizing unsupervised losses at prediction time, with theoretical guarantees and broad potential applications.
2. Formulating *meta-tailoring*, which adjusts the outer objective to optimize only the task loss, and developing a new algorithm, CNGRAD, for efficient meta-tailoring.
3. Demonstrating *tailoring* in 3 domains: encoding hard and soft conservation laws in physics prediction problems (Sec. 5.1 and Sec. 5.2), enhancing resistance to adversarial examples by increasing local smoothness at prediction time (Sec. 5.4), and improving prediction quality both theoretically (Sec. 3.1) and empirically (Sec. 5.3) by tailoring with a contrastive loss.

2 Related work

Tailoring is inspired by transductive learning. However, transductive methods, because they operate on a batch of unlabeled queries, are allowed to make use of the underlying distributional properties of those queries. In contrast, tailoring does the bulk of the computations before receiving any query; vastly increasing efficiency. Similar to tailoring, local learning [9] also has input-dependent parameters. However, it uses similarity in raw input space to select a few labeled data points and builds a local model instead of reusing the global prior learned across the whole data. Finally, some methods [20, 32] in meta-learning propagate predictions along the test samples in a semi-supervised transductive fashion.

Similar to tailoring, there are other learning frameworks that perform optimization at prediction time for very different purposes. Among those, energy-based models do generative modeling [2, 26, 31] by optimizing the hidden activations of neural networks, and other models [4, 47] learn to solve optimization problems by embedding optimization layers in neural networks, whose outputs are the solution of an optimization problem defined by the previous layer. In contrast, tailoring applies to the classic ML setting and instead optimizes the parameters of the model, not the hidden activations or the output.

As discussed in the introduction, unsupervised fine-tuning methods have been proposed to adapt to different types of variations between training and testing. Sun et al. [44] propose to adapt to a change of distribution with few samples by unsupervised fine-tuning at test-time, applying it with a loss of predicting whether the input has been rotated. Zhang et al. [52] build on it to adapt to group distribution shifts with a learned loss. Other methods in the few-shot meta-learning setting exploit test samples of a new task by minimizing either entropy [15] or a learned loss [5] in the inner optimization. Finally, Wang et al. [49] use entropy in the inner optimization to adapt to large-scale variations in image segmentation. In contrast, we propose (meta-)tailoring as a general effective way to impose inductive biases in the classic machine learning setting. Whereas in the aforementioned methods adaptation happens from training to testing, we independently adapt to every single query.

As discussed in the introduction, meta-learning [42, 7, 46, 27] has the same two-level optimization structure as meta-tailoring but focuses on multiple prediction tasks, each of which has its own separate training data. Because of this connection, most optimization-based meta-learning algorithms can be converted to the meta-tailoring setting. This is especially clear in the case of MAML [18] when we let the tailoring adaptation be a step of gradient descent:

$$\tau(\hat{\theta}, \mathcal{L}^{\text{tailor}}, x) = \hat{\theta} - \lambda \nabla_{\hat{\theta}} \mathcal{L}^{\text{tailor}}(x, \hat{\theta}).$$

Similar to CNGRAD, there are other optimization-based approaches to meta-learning whose adaptations can be batched [53, 39, 3]. Among these, [53, 40] train FiLM networks [38] to predict customized conditional normalization (CN) layers for each task. By optimizing the CN layers directly, CNGRAD is simpler, while remaining provably sufficiently expressive (section 4). More importantly, we can take an already trained model and add CNGRAD a posteriori by including CN layers with weights initialized to the identity.

3 Theoretical motivations of meta-tailoring

In this section, we study the potential advantages of meta-tailoring from the theoretical viewpoint, formalizing the intuitions conveyed in the introduction. By acting symmetrically during training and prediction time, meta-tailoring allows us to closely relate its training and expected losses, whereas tailoring, in general, may make them less related. First, we analyze the particular case of a contrastive tailoring loss. Then, we will generalize the guarantees to other types of tailoring losses.

3.1 Meta-tailoring with a contrastive tailoring loss

Contrastive learning [23] has seen significant successes recently in problems of semi-supervised learning from images [36, 25, 12]. The main idea is to create multiple versions of each training image and learn a representation in which variations of the same image are close while variations of different images are far apart. Typical augmentations involve cropping, color distortions, and rotation. We show theoretically that, under reasonable conditions, meta-tailoring using a particular contrastive loss $\mathcal{L}_{\text{cont}}$ as $\mathcal{L}^{\text{tailor}} = \mathcal{L}_{\text{cont}}$ helps us improve generalization errors in expectation compared with performing classical inductive learning.

When using meta-tailoring, we define $\theta_{x,S}$ to be the θ_x obtained with a training dataset $S = ((x_i, y_i))_{i=1}^n$ and tailored with the contrastive loss at the prediction point x. Theorem 1 provides an up-

per bound on the expected supervised loss $\mathbb{E}_{x,y}[\mathcal{L}^{\text{sup}}(f_{\theta_{x,S}}(x), y)]$ in terms of the expected contrastive loss $\mathbb{E}_x[\mathcal{L}_{\text{cont}}(x, \theta_{x,S})]$ (defined and analyzed in more detail in App. B), the empirical supervised loss $\frac{1}{n}\sum_{i=1}^{n} \mathcal{L}^{\text{sup}}(f_{\theta_{x_i,S}}(x_i), y_i)$ of meta-tailoring, and its uniform stability ζ. As a complement, instead of using the uniform stability ζ, Theorem 6 (App. C) provides a similar bound with the Rademacher complexity [6] $\mathcal{R}_n(\mathcal{L}^{\text{sup}} \circ \mathcal{F})$ of the set $\mathcal{L}^{\text{sup}} \circ \mathcal{F} = \{(x, y) \mapsto \mathcal{L}^{\text{sup}}(f_{\theta_x}(x), y) : (x \mapsto f_{\theta_x}(x)) \in \mathcal{F}\}$. Proofs of all results in this paper are deferred to App. C.

Definition 1. Let $S = ((x_i, y_i))_{i=1}^n$ and $S' = ((x'_i, y'_i))_{i=1}^n$ be any two training datasets that differ by a single point. Then, a meta-tailoring algorithm $S \mapsto f_{\theta_{\mathbf{x},S}}(x)$ is *uniformly ζ-stable* if $\forall (x, y) \in \mathcal{X} \times \mathcal{Y},\ |\mathcal{L}^{\text{sup}}(f_{\theta_{\mathbf{x},S}}(x), y) - \mathcal{L}^{\text{sup}}(f_{\theta_{\mathbf{x},S'}}(x), y)| \leq \frac{\zeta}{n}$.

Theorem 1. *Let $S \mapsto f_{\theta_{\mathbf{x},S}}(x)$ be a uniformly ζ-stable meta-tailoring algorithm. Then, for any $\delta > 0$, with probability at least $1 - \delta$ over an i.i.d. draw of n i.i.d. samples $S = ((x_i, y_i))_{i=1}^n$, the following holds: for any $\kappa \in [0, 1]$, $\mathbb{E}_{x,y}[\mathcal{L}^{\text{sup}}(f_{\theta_{\mathbf{x},S}}(x), y)] \leq \kappa \mathbb{E}_x \left[\mathcal{L}_{\text{cont}}(x, \theta_{\mathbf{x},S})\right] + (1 - \kappa)\mathcal{J}$, where $\mathcal{J} = \frac{1}{n}\sum_{i=1}^{n} \mathcal{L}^{\text{sup}}(f_{\theta_{\mathbf{x}_i,S}}(x_i), y_i) + \frac{\zeta}{n} + (2\zeta + c)\sqrt{(\ln(1/\delta))/(2n)}$, and c is the upper bound on the per-sample loss as $\mathcal{L}^{\text{sup}}(f_\theta(x), y) \leq c$.*

In the case of regular inductive learning, we get a bound of the exact same form, except that we have a single θ instead of a $\theta_{\mathbf{x}}$ tailored to each input x. These differences are marked in bold green in Definition 1 and Theorem 1. This theorem illustrates the effect of meta-tailoring on contrastive learning, with its potential reduction of the expected contrastive loss $\mathbb{E}_x[\mathcal{L}_{\text{cont}}(x, \theta_{x,S})]$. In classic induction, we may aim to minimize the empirical contrastive loss $\frac{1}{\bar{n}}\sum_{i=1}^{\bar{n}} \mathcal{L}_{\text{cont}}(x_i, \theta)$ with $\bar{n}$ potentially unlabeled training samples (in addition to the empirical supervised loss), which incurs the additional generalization error of $\mathbb{E}_x[\mathcal{L}_{\text{cont}}(x, \theta_{x,S})] - \frac{1}{\bar{n}}\sum_{i=1}^{\bar{n}} \mathcal{L}_{\text{cont}}(x_i, \theta)$. In contrast, meta-tailoring can avoid this extra generalization error by directly minimizing $\mathbb{E}_x[\mathcal{L}_{\text{cont}}(x, \theta_{x,S})]$.

In the case where $\mathbb{E}_x[\mathcal{L}_{\text{cont}}(x, \theta_{x,S})]$ is left large (e.g., due to large computational cost at prediction time), Theorem 1 still illustrates competitive generalization bounds of meta-tailoring with small κ, when compared to classical induction. For example, with $\kappa = 0$, it provides standard types of generalization bounds with the uniform stability for meta-tailoring algorithms. Even in this case, the bounds are not equivalent to those of classic induction, and there are potential benefits of meta-tailoring, which are discussed in the following section with a more general setting.

3.2 Meta-tailoring with general tailoring losses

The benefits of meta-tailoring go beyond contrastive learning: below we provide generalization bounds for meta-tailoring with any tailoring loss $\mathcal{L}^{\text{tailor}}(x, \theta)$ and any supervised loss $\mathcal{L}^{\text{sup}}(f_\theta(x), y)$.

Remark 1. *For any function φ such that $\mathbb{E}_{x,y}[\mathcal{L}^{\text{sup}}(f_\theta(x), y)] \leq \mathbb{E}_x[\varphi(\mathcal{L}^{\text{tailor}}(x, \theta))]$, Theorems 1 and 6 hold with the map $\mathcal{L}_{\text{cont}}$ being replaced by the function $\varphi \circ \mathcal{L}^{\text{tailor}}$.*

This remark shows the benefits of meta-tailoring through its effects on three factors: the expected unlabeled loss $\mathbb{E}_x[\varphi(\mathcal{L}^{\text{tailor}}(x, \theta_{x,S}))]$, uniform stability ζ, and the Rademacher complexity $\mathcal{R}_n(\mathcal{L}^{\text{sup}} \circ \mathcal{F})$. It is important to note that meta-tailoring can directly minimize the expected unlabeled loss $\mathbb{E}_x[\varphi(\mathcal{L}^{\text{tailor}}(x, \theta_{x,S}))]$, whereas classic induction can only minimize its empirical version, which results in the additional generalization error on the difference between the expected unlabeled loss and its empirical version. For example, if φ is monotonically increasing and $\mathcal{L}^{\text{tailor}}(x, \theta)$ represents the physical constraints at each input x (as in the application in section 5.1), then classic induction requires the physical constraints of neural networks at the *training* points to generalize to the physical constraints at *unseen* (e.g., testing) points. Meta-tailoring avoids this requirement by directly minimizing violations of the physical constraints at each point at prediction time.

Meta-tailoring can also improve the *parameter stability* ζ_θ defined such that $\forall (x, y) \in \mathcal{X} \times \mathcal{Y}, \|\theta_{x,S} - \theta_{x,S'}\| \leq \frac{\zeta_\theta}{n}$, for all S, S' differing by a single point. When $\theta_{x,S} = \hat{\theta}_S - \lambda \nabla \mathcal{L}^{\text{tailor}}(x, \hat{\theta}_S)$, we obtain an improvement on the parameter stability ζ_θ if $\nabla \mathcal{L}^{\text{tailor}}(x, \hat{\theta}_S)$ can pull $\hat{\theta}_S$ and $\hat{\theta}_{S'}$ closer so that $\|\theta_{x,S} - \theta_{x,S'}\| < \|\hat{\theta}_S - \hat{\theta}_{S'}\|$, which is ensured, for example, if $\|\cdot\| = \|\cdot\|_2$ and $\text{cos_dist}(v_1, v_2)\frac{\|v_1\|}{\|v_2\|} > \frac{1}{2}$ where $\text{cos_dist}(v_1, v_2)$ is the cosine similarity of v_1 and v_2, with $v_1 = \hat{\theta}_S - \hat{\theta}_{S'}$, $v_2 = \lambda(\nabla \mathcal{L}^{\text{tailor}}(x, \hat{\theta}_S) - \nabla \mathcal{L}^{\text{tailor}}(x, \hat{\theta}_{S'}))$ and $v_2 \neq 0$. Here, the uniform stability ζ and the parameter stability ζ_θ are closely related as $\zeta \leq C\zeta_\theta$, where C is the upper bound on the Lipschitz constants of the maps $\theta \mapsto \mathcal{L}^{\text{sup}}(f_\theta(x), y)$ over all $(x, y) \in \mathcal{X} \times \mathcal{Y}$ under the norm $\|\cdot\|$, since $|\mathcal{L}^{\text{sup}}(f_{\theta_{x,S}}(x), y) - \mathcal{L}^{\text{sup}}(f_{\theta_{x,S'}}(x), y)| \leq C\|\theta_{x,S} - \theta_{x,S'}\| \leq \frac{C\zeta_\theta}{n}$.

4 CNGRAD: a simple algorithm for expressive, efficient (meta-)tailoring

In this section, we address the issue of using (meta-)tailoring for efficient GPU computations. Whereas one can efficiently parallelize the evaluation of a single model over a batch across inputs, it can be challenging to efficiently parallelize the evaluation of multiple *tailored* models over a batch. To overcome this issue, building on CAVIA [53] and WarpGrad [19], we propose CNGRAD which adapts only *conditional normalization* parameters and enables efficient GPU computations for (meta-)tailoring. CNGRAD can also be used in regular meta-learning; details and pseudo-codes of both versions are in App. D.

As is done in batch-norm [29] after element-wise normalization, we can implement an element-wise affine transformation with parameters (γ, β), scaling and shifting the output $h_k^{(l)}(x)$ of each k-th neuron at the l-th hidden layer independently: $\gamma_k^{(l)} h_k^{(l)}(x) + \beta_k^{(l)}$. In conditional normalization, Dumoulin et al. [17] train a collection of (γ, β) in a multi-task fashion to learn different tasks with a single network. CNGRAD brings this concept to meta-learning and (meta-)tailoring settings and adapts the affine parameters (γ, β) to each query. For meta-tailoring, the inner loop minimizes the tailoring loss at an input x by adjusting the affine parameters and the outer optimization adapts the rest of the network. Similar to MAML [18], we implement a first-order version, which does not back-propagate through the optimization, and a second-order version, which does. CNGRAD efficiently parallelizes computations of multiple tailored models over a (mini-)batch in a GPU, because the adapted parameters only require element-wise multiplications and additions.

CNGRAD is widely applicable since the adaptable affine parameters can be added to any hidden layer, and only represent a tiny portion of the network (empirically, 1%). Moreover, we can that, under realistic assumptions, we can minimize the inner tailoring loss using only the affine parameters. To analyze properties of these adaptable affine parameters, let us decompose θ into $\theta = (w, \gamma, \beta)$, where w contains all the weight parameters (including bias terms), and the (γ, β) contains all the affine parameters. Given arbitrary coefficients $\eta_1, \ldots, \eta_{n_g} \in \mathbb{R}$ and an arbitrary function $(f_\theta(x), x) \mapsto \ell_{\text{tailor}}(f_\theta(x), x)$, let $\mathcal{L}^{\text{tailor}}(x, \theta) = \sum_{i=1}^{n_g} \eta_i \ell_{\text{tailor}}(f_\theta(g^{(i)}(x)), x)$, where $g^{(1)}, \ldots, g^{(n_g)}$ are arbitrary input augmentation functions at prediction time. Note that n_g is typically small ($n_g \ll n$) in meta-tailoring; e.g., $n_g = 1$ in the method in Section 5.1 regardless of the size of the dataset n.

Corollary 1 states that for any given $\hat{w}$, if we add any non-degenerate Gaussian noise δ as $\hat{w} + \delta$ with zero mean and any variance on δ, the global minimum value of $\mathcal{L}^{\text{tailor}}$ w.r.t. all parameters (w, γ, β) can be achieved by optimizing only the affine parameters (γ, β), with probability one.

Assumption 1. *(Common activation)* The activation function $\sigma(x)$ is real analytic, monotonically increasing, and the limits exist as: $\lim_{x \to -\infty} \sigma(x) = \sigma_- > -\infty$ and $\lim_{x \to +\infty} \sigma(x) = \sigma_+ \leq +\infty$.

Theorem 2. *For any $x \in \mathcal{X}$ that satisfies $\|g^{(i)}(x)\|_2^2 - g^{(i)}(x)^\top g^{(j)}(x) > 0$ (for all $i \neq j$), and for any fully-connected neural network with a single output unit, at least n_g neurons per hidden layer, and activation functions that satisfy Assumption 1, the following holds: $\inf_{w,\gamma,\beta} \mathcal{L}^{\text{tailor}}(x, w, \gamma, \beta) = \inf_{\gamma,\beta} \mathcal{L}^{\text{tailor}}(x, \bar{w}, \gamma, \beta)$ for any $\bar{w} \notin \mathcal{W}$ where Lebesgue measure of $\mathcal{W} \subset \mathbb{R}^d$ is zero.*

Corollary 1. *Under the assumptions of Theorem 2, for any $\hat{w} \in \mathbb{R}^d$, with probability one over randomly sampled $\delta \in \mathbb{R}^d$ accordingly to any non-degenerate Gaussian distribution, the following holds: $\inf_{w,\gamma,\beta} \mathcal{L}^{\text{tailor}}(x, w, \gamma, \beta) = \inf_{\gamma,\beta} \mathcal{L}^{\text{tailor}}(x, \hat{w} + \delta, \gamma, \beta)$ for any $x \in \mathcal{X}$.*

The assumption and condition in theorem 2 are satisfied in practice (see App. A). Therefore, CNGRAD is a practical and computationally efficient method to implement (meta-)tailoring.

5 Experiments

5.1 Tailoring to impose symmetries and constraints at prediction time

Exploiting invariances and symmetries is an established strategy for increasing performance in ML. During training, we can regularize networks to satisfy certain criteria; but this doesn't guarantee they will be satisfied outside the training dataset [43]. (Meta-)tailoring provides a general solution to this problem by adapting the model at prediction time to satisfy the criteria. We demonstrate the use of tailoring to enforce physical conservation laws for predicting the evolution of a 5-body planetary system. This prediction problem is challenging, as m-body systems become chaotic for $m > 2$. We generate a dataset with positions, velocities, and masses of all 5 bodies as inputs and the changes in position and velocity as targets. App. E further describes the dataset.

Method	loss	relative
Inductive learning	.041	-
Opt. output(50 st.)	.041	$(0.7 \pm 0.1)\%$
6400-s. TTT(50 st.)	.040	$(3.6 \pm 0.2)\%$
Tailoring(1 step)	.040	$(1.9 \pm 0.2)\%$
Tailoring(5 steps)	.039	$(6.3 \pm 0.3)\%$
Tailoring(10 st.)	.038	$(7.5 \pm 0.1)\%$
Meta-tailoring(0 st.)	.030	$(26.3 \pm 3.3)\%$
Meta-tailoring(1 st.)	.029	$(29.9 \pm 3.0)\%$
Meta-tailoring(5 st.)	.027	$(35.3 \pm 2.6)\%$
Meta-tailoring(10 s.)	.026	$(36.0 \pm 2.6)\%$

Table 1: Test MSE loss for different methods; the second column shows the relative improvement over basic inductive supervised learning. The test-time training (TTT) baseline uses a full batch of 6400 test samples to adapt, not allowed in regular SL. With a few gradient steps, tailoring significantly over-performs all baselines. Meta-tailoring improves even further, with 35% improvement.

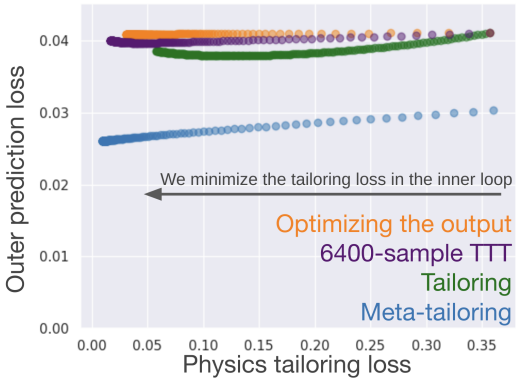

Figure 2: Optimization at prediction time on the planet data; each path going from right to left as we minimize the physics tailoring loss. We use a small step size to illustrate the path. Tailoring and the two baselines only differ in their test-time computations, thus sharing their starts. Meta-tailoring has a lower starting loss, faster optimization, and no overfitting during tailoring.

Our model is a 3-layer feed-forward network. We tailor it by taking the original predictions and adapting the model using the tailoring loss which is given by the L_1 loss between the initial and final energy and momentum of the whole system. Note that ensuring this conservation doesn't guarantee better performance: predicting the input as output conserves energy and momentum perfectly, but is not correct.

While tailoring adapts some parameters in the network to improve the tailoring loss, an alternative for enforcing conservation would be to adapt the output y value directly. Table 1 compares the predictive accuracy of inductive learning, direct output optimization and both tailoring and meta-tailoring, using varying numbers of gradient steps. Tailoring is more effective than adapting the output, as the parameters provide a prior on what changes are more natural. For meta-tailoring, we try both first-order and second-order versions of CNGRAD: the first-order gave slightly better results, possibly because it was trained with a higher tailor learning rate (10^{-3}) with which the second-order version was unstable (we thus used 10^{-4}). More details can be found in App. E.

Finally, meta-tailoring without any query-time tailoring steps already performs much better than the original model, even though both have almost the same number of parameters and can overfit the dataset. We conjecture meta-tailoring training adds an inductive bias that guides optimization towards learning a more generalizable model. Fig. 2 shows prediction-time optimization paths.

5.2 Tailoring to softly encourage inductive biases

A popular way of encoding inductive biases is with clever network design to make predictions translation equivariant (CNNs), permutation equivariant (GNNs), or conserve energy [22]. However, if an inductive bias is only partially satisfied, such approaches overly constrain the function class. Tailoring instead can softly impose this bias by only fine-tuning the corresponding tailoring loss for a few steps.

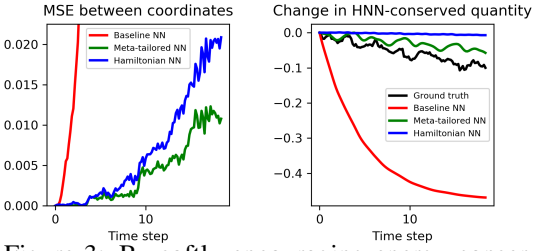

Figure 3: By softly encouraging energy conservation, meta-tailoring improves over models that don't and models that fully impose it.

We showcase this in the real pendulum experiment used by Hamiltonian Neural Networks (HNNs) [22]. HNNs have energy conservation built-in, and easily improve a vanilla MLP. We meta-tailor this vanilla MLP with energy conservation, without changing its architecture. Meta-tailoring significantly improves over the baseline and HNNs, since it can encode the *imperfect* energy conservation of real systems. We compare results in Fig. 3 and provide extra details in App. F.

σ	**Method**	0.0	0.5	1.0	1.5	2.0	2.5	3.0	ACR
0.25	(Inductive) Randomized Smoothing	0.67	0.49	0.00	0.00	0.00	0.00	0.00	0.470
	Meta-tailored Randomized Smoothing	**0.72**	**0.55**	0.00	0.00	0.00	0.00	0.00	**0.494**
0.50	(Inductive) Randomized Smoothing	0.57	0.46	0.37	0.29	0.00	0.00	0.00	0.720
	Meta-tailored Randomized Smoothing	0.66	0.54	**0.42**	**0.31**	0.00	0.00	0.00	**0.819**
1.00	(Inductive) Randomized Smoothing	0.44	0.38	0.33	0.26	0.19	0.15	0.12	0.863
	Meta-tailored Randomized Smoothing	0.52	0.45	0.36	**0.31**	**0.24**	**0.20**	**0.15**	**1.032**

Table 2: Percentage of points with certificate above different radii, and ACR for ImageNet. Meta-tailoring improves ACR by $5.1\%, 13.8\%, 19.6\%$. Results for Cohen et al. [13] are taken from [51].

Note that, with inexact losses, fully enforcing them provides sub-optimal results. Thus, we pick the tailoring learning rate that results in the lowest long-term prediction loss during training.

5.3 Tailoring with a contrastive loss for image classification

Following the setting described in section 3.2, we provide experiments on the CIFAR-10 dataset [30] by building on SimCLR [12]. SimCLR trains a ResNet-50 [24] $f_\theta(\cdot)$ coupled to a small MLP $g(\cdot)$ such that the outputs of two augmentations of the same image $x_i, x_j \sim \mathcal{T}(x)$ agree; i.e. $g(f_\theta(x_i)) \approx g(f_\theta(x_j))$. This is done by training $g(f(\cdot))$ to recognize one augmentation from the other among a big batch of candidates with the cross-entropy loss. To show that the unsupervised training of f_θ provides a useful representation, SimCLR trains a single linear layer on top of it, $\phi(f_\theta(\cdot))$, achieving good classification results.

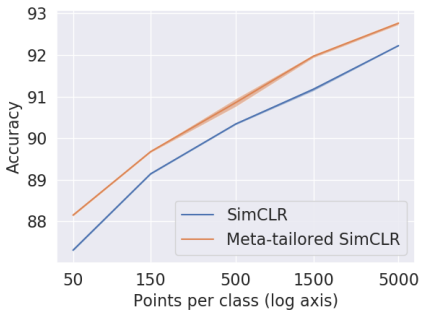

Figure 4: Meta-tailoring the linear layer with the contrastive loss results in consistent gains between 0.5% and 0.8% in accuracy. This is approximately the same gain as that of doubling the amount of labeled data (note the logarithmic x-axis).

Building on SimCLR, tailoring f_θ at prediction-time by optimizing $g(f_{\theta_x}(x))$ maximizes agreement between augmentations. At train time, meta-tailoring doesn't redo SimCLR unsupervised learning, which provides θ. Its outer loop only trains ϕ to take the tailored representations $f_{\theta_x}(x)$. Thus, θ is unsupervisedly fine-tuned in the prediction function leading to θ_x, but never supervisedly trained as this would break the evaluation protocol (in meta-tailoring's favor). Results in Fig. 4, TTT [44] performed worse than base SimCLR (see App.).

5.4 Tailoring for robustness against adversarial examples

Neural networks are susceptible to adversarial examples [8, 45]: targeted small perturbations of an input can cause the network to misclassify it. One approach is to make the prediction function smooth via adversarial training [33]; however, this only ensures smoothness in the training points. Constraining the model to be smooth everywhere makes it lose capacity. Instead, (meta-)tailoring asks for smoothness *a posteriori*, only on a specific query.

We apply meta-tailoring to robustly classifying CIFAR-10 [30] and ImageNet [14] images, tailoring predictions so that they are locally smooth. Inspired by the notion of adversarial examples being caused by predictive, but non-robust, features [28], we meta-tailor our model by enforcing smoothness on the vector of features of the penultimate layer (denoted $g_\theta(x)$):

$$\mathcal{L}^{\text{tailor}}(x, \theta) = \mathbb{E}[\text{cos_dist}(g_\theta(x), g_\theta(x + \delta))], \delta \sim N(0, \nu^2),$$

We build on Cohen et al. [13], who developed a method for certifying the robustness of a model via randomized smoothing (RS). RS samples points from a Gaussian $N(x, \sigma^2)$ around the query and, if there is enough agreement in classification, it provides a certificate that the query cannot be adversarially modified by a small perturbation to have a different class. We show that meta-tailoring improves the original RS method, testing for $\sigma = 0.25, 0.5, 1.0$. We use $\nu = 0.1$ for all experiments. We initialized with the weights of Cohen et al. [13] by leveraging that CNGRAD can start from a pre-trained model by initializing the extra affine layers to the identity. Finally, we use $\sigma' = \sqrt{\sigma^2 - \nu^2} \approx 0.23, 0.49, 0.995$ so that the points used in our tailoring loss come from $N(x, \sigma^2)$.

Table 6 shows our results on CIFAR-10 where we improve the average certification radius (ARC) by $8.6\%, 10.4\%, 19.2\%$ respectively. In table 2, we show results on Imagenet where we improve the ARC by $5.1\%, 13.8\%, 19.6\%$ respectively. We chose to meta-tailor the RS method because it represents a strong standard in certified adversarial defenses, but we note that there have been advances on RS that sometimes achieve better results than those presented here [51, 41], see App. H. However, likely, meta-tailoring can also improve these methods.

These experiments only scratch the surface of what tailoring allows for adversarial defenses: usually, the adversary looks at the model and gets to pick a particularly bad perturbation $x + \delta$. With tailoring, the model responds, by changing to weights $\theta_{x+\delta}$. This leads to a game, where both weights and inputs are perturbed, similar to $\max_{|\delta|<\epsilon_x} \min_{|\Delta|<\epsilon_\theta} \mathcal{L}^{\text{sup}}\left(f_{\theta+\Delta}(x+\delta), y\right)$. However, since we don't get to observe y; we optimize the weight perturbation by minimizing $\mathcal{L}^{\text{tailor}}$ instead.

6 Discussion

6.1 Broader Impact

Improving adversarial robustness: having more robust and secure ML systems is mostly a positive change. However, improving adversarial defenses could also go against privacy preservation. Encoding desirable properties: By optimizing an unsupervised loss for the particular query we care about, it is easier to have guarantees on the prediction. In particular, there could be potential applications for fairness, where the unsupervised objective could enforce specific criteria at the query or related inputs. More research needs to be done to make this assertion formal and practical. Potential effect on privacy: tailoring specializes the model to each input. This could have an impact on privacy. Intuitively, the untailored model can be less specialized to each input, lowering the individual information from each training point contained in the model. However, tailored predictions have more information about the queries, from which more personal information could be leaked.

6.2 Limitations

Tailoring provides a framework for encoding a wide array of inductive biases, but these need to be specified as a formula by the user. For instance, it would be hard to codify tailoring losses in raw pixel data, such as mass conservation in pixel space. Tailoring also incurs an extra time cost at prediction time, since we make an inner optimization inside the prediction function. However, as shown in Table 1, meta-tailoring often achieves better results than inductive learning even without adaptation at test-time, enabling predictions at regular speed during test-time. This is due to meta-tailoring leading to better training. Moreover, optimization can be sped up by only tailoring the last layers, as discussed in App. D. Finally, to the best of our knowledge a naive implementation of tailoring would be hard to parallelize in PyTorch [37] and Tensorflow [1]; we proposed CNGRAD to make it easy and efficient. JAX[10], which better handles per-example weights, makes parallelizing tailoring effortless.

Theory in Sec. 3 applies only for meta-tailoring. Unlike tailoring (and test-time training), meta-tailoring performs the same computations at training and testing time, which allows us to prove the results. Theorem 2 proves that optimizing the CN layers in CNGRAD has the same expressive power as optimizing all the layers for the inner (not outer) loss. However, it does not guarantee that gradient descent will find the appropriate optima. The study of such guarantee is left for future work.

6.3 Conclusion

We have presented *tailoring*, a simple way of embedding a powerful class of inductive biases into models, by minimizing unsupervised objectives at prediction time. Tailoring leverages the generality of auxiliary losses and improves them in two ways: first, it eliminates the generalization gap on the auxiliary loss by optimizing it on the query point; second, tailoring only minimizes task loss in the outer optimization and the tailoring loss in the inner optimization. This results in the whole network optimizing the only objective we care about, instead of a proxy loss. Finally, we have formalized these intuitions by proving the benefits of meta-tailoring under mild assumptions.

Tailoring is broadly applicable, as one can vary the model, the unsupervised loss, and the task loss. We show its applicability in three diverse domains: physics prediction time-series, contrastive learning, and adversarial robustness. We also provide a simple algorithm, CNGRAD, to make meta-tailoring practical with little additional code. Currently, most unsupervised or self-supervised objectives without taking into account the supervised down-stream task. Instead, meta-tailoring provides a generic way to make these objectives especially useful for each particular application.

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1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes] In section 6.2.
   (c) Did you discuss any potential negative societal impacts of your work? [Yes] In section 6.1.
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes] Important assumptions are in the main text; all assumptions are detailed in the appendix, particularly in appendix A.
   (b) Did you include complete proofs of all theoretical results? [Yes] In appendix C.
3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [No] We plan, however, to open-source our codebase once cleaned.
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   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [No] We report them for the planet experiments and the contrastive experiments. The adversarial experiments are extremely computationally expensive and we only ran them once.
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