Learning (Local) Surrogate Loss Functions for Predict-Then-Optimize Problems

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Abstract

Decision-Focused Learning (DFL) is a paradigm for tailoring a predictive model to a downstream optimisation task that uses its predictions, so that it can perform better on that specific task. The main technical challenge associated with DFL is that it requires being able to differentiate through \( \text{argmin} \) operations to work. However, these \( \text{arg min} \) optimisations are often piecewise constant and, as a result, naively differentiating through them would provide uninformative gradients. Past work has largely focused on getting around this issue by handcrafting task-specific surrogates to the original optimisation problem that provide informative gradients when differentiated through. However, finding these surrogates can be challenging and the need to handcraft surrogates for each new task limits the usability of DFL. In addition, even after applying these relaxation techniques, there are no guarantees that the resulting surrogates are convex and, as a result, training a predictive model on them may lead to said model getting stuck in local minimas. In this paper, we provide an approach to learn faithful task-specific surrogates which (a) only requires access to a black-box oracle that can solve the optimisation problem and is thus generalizable, and (b) can be convex by construction and so can be easily optimized over. To the best of our knowledge, this is the first work on using learning to find good surrogates for DFL. We evaluate our approach on a budget allocation problem from the literature and find that our approach outperforms even the hand-crafted (non-convex) surrogate loss proposed by the original paper. Taking a step back, we hope that the generality and simplicity of our approach will help lower the barrier associated with implementing DFL-based solutions in practice. To that end, we are currently working on extending our experiments to more domains.

1 Introduction

Predict-Then-Optimize is a framework for decision-making under uncertainty. As the name suggests, it proceeds in two stages—first, a predictive model takes as input features and makes some predictions using them, then second, these predictions are used to parameterize an optimization problem that produces as output a set of decisions. A large number of real-world applications involve both prediction and optimisation components and can be framed as predict-then-optimize problems—for e.g., recommender systems in which missing user-item ratings need to be predicted [7], portfolio optimisation in which future performance needs to be predicted [10], or strategic decision-making in which the adversary behaviour needs to be predicted [8].
Historically, learning a predictive model was done independently of the downstream optimization task. However, recently there has been literature \cite{4, 9, 14, 5, 11, 14, 16, 15, 2} that shows that it is possible to achieve better task-specific performance by tailoring the predictive model to the downstream task. A large subset of the approaches to do this, which we will refer to as Decision-Focused Learning (DFL) \cite{14} in this paper, learn a good predictive model by differentiating through the prediction + optimization pipeline end-to-end. Differentiating through the optimisation problem to learn a good predictive model creates what we call the Decision Loss (DL), which optimizes for the quality of decisions induced by predictions.

However, differentiating through the optimization problem is challenging because the solutions to these optimization problems are often piecewise constant in the input predictions. For example, the optimization $\arg \min(\hat{y}_1, \hat{y}_2)$ that picks the smaller of two predicted values $\hat{y}_1$ and $\hat{y}_2$ doesn’t change its decision if the prediction was instead $\hat{y}_1 \pm \epsilon$ (unless the two predictions were very close to equal initially). When differentiating through such a problem, the gradients are either zero or undefined, neither of which are useful for learning a predictive model.

To address this challenge, there’s been significant recent research focused on finding good surrogate tasks that are both faithful to the original decision task, and also provide informative gradients for learning good predictive models. They typically do this by either finding ways to relax the optimization problem \cite{4, 9, 14, 5}, adding regularisation terms \cite{1, 14, 16}, or even creating entirely different surrogate problems \cite{15, 2}. However, these approaches tend to be handcrafted for specific optimization problems and cannot be readily generalized to new ones. In addition, even though these surrogates provide non-zero gradients, there are no guarantees that the resulting surrogates will be convex and, as a result, may lead to predictive models that are trained using them to get stuck in local optima.

The solution to these problems would be an approach that generates (1) faithful and (2) convex surrogates for (3) arbitrary optimisation tasks that help learn predictive models that (4) perform well on the downstream optimisation tasks. While this may be challenging in general, we make an assumption that allow us to simplify this challenge—we assume that our predictive model can get close to the true label but needs task-specific information to differentiate between nearby points. Consequently, our surrogate only has to be faithful in the neighbourhood of the true labels.

In this paper, we introduce an approach that learns surrogate loss functions that satisfy the properties above. Specifically, we use the assumption above to sample points in the neighbourhood of the ground truth labels, evaluate the DL associated with these sampled points, and then train a surrogate loss which is faithful to the decision loss. Our approach has two key advantages. First, we can choose the parametric family for the surrogate loss in order to guarantee desirable properties such as convexity (see Section 4.1). Second, it is highly generalizable because it only requires oracle calls to a black-box solver of the optimization problem. As a result, it satisfies 3 out of the 4 properties by design.

To evaluate the fourth criterion – performance – we present an initial set of experimental results on a ‘budget allocation’ task from Wilder et al. \cite{14}. Perhaps surprisingly, we find that our approach actually outperforms the handcrafted (but non-convex) DFL approach proposed by the paper. Specifically, we find that it consistently does well across multiple problem instances, while DFL appears prone to getting stuck in local minima. We also find that our surrogate function empirically satisfies additional desirable properties – it learns a similar structural relationship as the DFL approach (though more robustly), and its performance is directly correlated with how well it imitates the decision loss.

## 2 Related Work

This paper is motivated by the recent work on “Decision-Focused Learning” (DFL) \cite{14, 3} and the related literature—for e.g., “Smart Predict-Then-Optimize” \cite{4}. Elmachtoub and Grigas \cite{4} show how a predictive model that maximises the optimization objective can be different from one that maximises predictive accuracy, and propose a duality-based approach for learning such a “smart” predictive model. However, their approach is only applicable to optimization problems that can be framed as Linear Programs (LPs).
For more complex optimization problems, the DFL literature proposes learning such a “smart” predictive model by differentiating the prediction + optimization pipeline end-to-end. However, as we’ve seen above, differentiating through the arg min operation in Equation 1 isn’t straightforward. As a result, past work on DFL typically focuses on what the right surrogates (that provide informative gradients for learning good predictive models) to classes of optimization problems are [15][8][4][1][6][2].

There is also some work that discusses alternatives to DFL that don’t require coming up with custom relaxations to the optimization problems of interest. Mulamba et al. [11] provide a contrastive learning-based proxy objective that doesn’t require differentiating through (or even solving) the optimization problem \( z^*(\hat{y}) \). However, this approach makes a strong assumption about the nature of the decision loss \( DL \), while our approach can learn surrogates that are tailored to any optimization problem. Additionally, Sodhi et al. [13] propose an energy-based optimization method for learning a “smart” predictive model. However, their approach is fundamentally unsupervised and requires learning both a good predictive model and a good surrogate loss simultaneously. In this paper, we use the fact that we know and can exactly compute the loss that we’re trying to minimise (i.e., \( DL \)) to learn a surrogate loss independently of the predictive model.

Finally, there are also papers that try to learn global approximations to optimization problems like the AUC [6], or even those that try to solve hard optimization problems directly [12]. However, learning global approximations (i.e., for all possible \( y \)) is a much harder than learning local approximations (in the neighbourhood of a single \( y \)). This seems to be the first paper advocating the use of local surrogates.

3 Background

Decision-Focused Learning is a recent paradigm for formalising decision-making using machine learning. First, one looks at some features \( x \) and then, using a machine learning model \( M_\theta \) with parameters \( \theta \), makes some predictions \( \hat{y} = M_\theta(x) \) based on it. Second, these predictions \( \hat{y} \) are then used to parameterize an optimization problem \( z^*(\hat{y}) \), that solves for the best decision:

\[
z^*(\hat{y}) = \arg \min_n f(z, \hat{y}) \\
\text{s.t. } g_i(z) \leq 0 \quad \text{for } i \in \{1, \ldots, m\} \tag{1}
\]

Consequently, a set of predictions are ‘good’ if they lead to decisions that have good outcomes. Concretely, this ‘decision loss’ \( DL \) is given by how well the decisions \( z^*(\hat{y}) \) (made based on the predictions \( \hat{y} \)) perform in the ‘real’ world (that’s parameterized by the true labels \( y \)):

\[
DL(\hat{y}, y) = f(z^*(\hat{y}), y)
\]

where \( f \) is the objective of the optimization problem.

Then, for a dataset \( \{(x_1, y_1), \ldots, (x_N, y_N)\} \), the aim is to learn a model \( M_\theta \) that will generate predictions \( \{\hat{y}_1, \ldots, \hat{y}_N\} \) such that the expected decision loss is minimised over the observed data:

\[
\theta^* = \arg \min_\theta \frac{1}{N} \sum_{n=1}^{N} DL(M_\theta(x_n), y_n)
\]

This is in contrast with ‘traditional ML,’ in which the ‘goodness’ of a prediction is based on a somewhat ‘intermediate’ loss \( IL(\hat{y}, y) \) (e.g. Mean Squared-Error) that has no information about the downstream decision-making task.

Historically, the way in which past work (for e.g., [14]) has optimized for \( \theta \) is to backpropagate the errors through the decision-loss \( DL \) (which includes the computation of the optimal decision \( z^*(\hat{y}) \)) to \( M_\theta \). However, as we have noted in the introduction, differentiating through the arg min operation

\footnote{Note that \( M_\theta \) is in bold because, in general, it can be thought to take as input a set of features \( x \) and provides as output the set of all predictions \( \hat{y} \) needed to parameterize the optimization problem. However, in practice, there can be hundreds of relevant predictions \( y_i = [y_{i,0}, \ldots, y_{i,L}] \), each of which have an identical structure. In such cases, the problem is typically decomposed into learning a mapping \( M_\theta \) from each of \( x_{i,l} \in [x_{i,0}, \ldots, x_{i,L}] \) to an individual prediction \( y_{i,l} \in \hat{y} \).}
can be uninformative because $z^*$ is often piecewise constant. The broad strategy to overcome this is to come up with a ‘surrogate’ loss $SL$ that (a) induces decisions that perform well on $DL$, and (b) provides informative gradients. In addition, it is desirable for $SL$ to have convexity properties so that, when $M_0$ is trained using $SL$ using gradient descent, it doesn’t get stuck in any local minima.

4 Our Approach

In this paper, we attempt to get around the problem of having to find custom task-specific relaxations of the optimization problem $z^*(\hat{y})$ by instead learning a surrogate loss $SL_\phi(\hat{y}, y)$ (parameterized by $\phi$) that approximates the behaviour of $DL$ and has nice convexity properties.

4.1 Learning and Using $SL_\phi$

Then, to learn $SL_\phi$, for some set of true labels $y_n$ from the dataset, we proceed in two steps:

(Step 1) Sample Points:

We sample a set of $K$ points $[y_n^1, \ldots, y_n^K]$ in the vicinity of $y$ and calculate $DL(y_n^k, y_n)$ for each. In this paper, we consider 3 sampling strategies:

1. All-Perturbed: In this version of the problem, a data point is generated by adding zero-mean Gaussian noise to the true label $y_n$:

   $$y_n^k = y_n + \epsilon^k = y_n + \alpha \cdot \mathcal{N}(0, I)$$

   where, $\alpha$ is a normalisation factor and $I$ is a $dim(y) \times dim(y)$ identity matrix.

2. 1-Perturbed or 2-Perturbed: In a way, trying to estimate the behaviour of $DL(y_n + \epsilon^i, y_n)$ for small $\epsilon_i$ is similar to trying to calculate $(\frac{\partial}{\partial y_n})^{dim(y_n)} DL(\hat{y}_n, y_n)$ (i.e. the $dim(y_n)$th partial derivative of $DL$ wrt its first input $\hat{y}_n$) at $(y_n, y_n)$ because all the dimensions of $\hat{y}_n$ are being varied simultaneously. While doing this is hard, perhaps a good approximation for it is the 1st or 2nd partial derivative. Then, the way to numerically calculate the Jacobian and Hessian is to perturb only one or two dimensions at a time (and then fit an appropriate model to it, like the “Quadratic” model below).

(Step 2) Fit Surrogate Loss:

We use the dataset created above to fit a surrogate loss function $SL_\phi(y_n^i) \approx SL(y_n^i, y_n)$ such that the mean squared error is minimised:

$$\phi^*_n = \arg \min_{\phi_n} \frac{1}{K} \sum_{k=1}^K (SL_\phi(y_n^k) - DL(y_n^k, y_n))^2$$

In this paper, we consider 3 families of loss functions for $SL_\phi$:

1. NN: In which $SL_\phi$ is parameterized as a full-connected (3-layer) Neural Network (NN) such that $SL_\phi = NN_\phi(\hat{y})$. This is, in some sense, the ‘naive’ learning-based solution. However, one possible issue with this approach is that, if we’re modelling a loss function using an NN, there’s no guarantee about what the ‘minima’ of said loss function will be. (This leads to instability in practice, as we see in the experiments.)

2. Weighted-MSE: In which $SL_\phi$ is parameterized as a weighted version of MSE $(\sum_{l=1}^{dim(y)} w_l \cdot (\hat{y}_l - y_l)^2)$ such that the ‘weights’ $w_l$ associated with different predictions are what’s learned. This is another ‘obvious’ choice – MSE is a popular 2-stage regression loss, and has nice properties (its minima is the true label $y_n$ and it’s convex). In addition, the weights allow us to learn which dimensions of $y$ are more important than others based on the optimization task.

3. Quadratic: In which $SL_\phi$ is parameterized as $(\hat{y} - y)^T H (\hat{y} - y)$, where $H$ is a learned low-rank symmetric PSD matrix. This family of functions has 2 desirable properties: (1) its minima is $y$ by definition, and (2) it is convex (as long as $H$ is PSD). Accordingly, this is the approach we expect to perform best. It also has an appealing interpretation inspired by the idea above, that learning a ‘local’ surrogate is similar to estimating the
partial derivative of $DL$ with respect to its first input $\hat{y}_n$. Specifically, if we look at the first 3 terms of the Taylor expansion of $DL$ with respect to $\hat{y}_n$ at $(y_n, y_n)$, we get:

$$
\frac{\partial}{\partial \hat{y}_n} DL(y_n + e, y_n) = \frac{\partial}{\partial \hat{y}_n} DL(y_n, y_n) + \nabla_{\hat{y}_n} DL(y_n, y_n) e + \epsilon^T \nabla^2_{\hat{y}_n} DL(y_n, y_n) e + \ldots
$$

$$
\approx DL(y_n, y_n) + (\hat{y}_n - y_n)^T H(\hat{y}_n - y_n)
$$

So, our Quadratic $SL_\phi$ can be seen as a 2nd-order Taylor-series approximation of $DL$ at $(y_n, y_n)$ where our learned $H$ tries to approximate the Hessian of $DL$. We are missing the $DL(y_n, y_n)$ term, but given that $SL_\phi$ is a loss function that we’re optimising over, the subtraction of a constant doesn’t affect the gradients passed to $M_\theta$.

(Step 3) Train $M_\theta$ using $SL_\phi$:

Given this surrogate loss $SL_\phi$ from Step 2, the predictive model is trained such that:

$$
\theta^* = \arg\min_\theta \frac{1}{N} \sum_{n=1}^{N} SL_{\phi_n}(M_\theta(x_n), y_n)
$$

$$
\approx \arg\min_\theta \frac{1}{N} \sum_{n=1}^{N} DL(M_\theta(x_n), y_n)
$$

(2)

4.2 Simplifications for Learning $SL_\phi$

In Equation [2] we refer to $SL_{\phi_n}$ rather than the more general $SL_\phi$. This is because we learn a different $SL_{\phi_n}$ for every $[(x_1, y_1), \ldots, (x_n, y_n), \ldots, (x_N, y_N)]$. We make this distinction here because learning a global approximation to $DL(\hat{y}, y)$ (for arbitrary $\hat{y}$) is hard; it boils down to learning a closed-form approximation to the general optimization problem $z^*(\hat{y})$.

Instead, we simplify our lives in two ways in this paper:

1. Learning for a specific $y_n$: Instead of learning a $\mathbb{R}^{\text{dim}(y)+\text{dim}(\hat{y})}$ function $SL_\phi(\hat{y}, y)$ to imitate $DL(\hat{y}, y)$, we instead learn $N$ different $\mathbb{R}^{\text{dim}(\hat{y})}$ functions $SL_{\phi_n}(\hat{y})$ that imitate $DL(\hat{y}, y_n)$ for each $n \in N$.

   One benefit of doing this is that it reduces the dimensionality of the learning problem – this is especially relevant when $N$ is not very large in comparison to $\text{dim}(y)$ (as in our experiments). However, in addition, it also removes the need to account for invariances baked into the more general learning problem – for example, permutations of $y$ and $\hat{y}$ should produce the same output for the task we consider, but enforcing this constraint is tricky. Instead, when the ordering of $y$ is fixed, this is no longer cause for concern.

2. Learning for only $\hat{y}_n \approx y_n$: In addition to the simplification above, we don’t try to learn a faithful approximation $\forall \hat{y} \in \mathbb{R}^{\text{dim}(y)}$, we instead limit ourselves to learning an approximation of $DL(\hat{y}, y_n)$ only when $\hat{y}$ is in the neighbourhood of $y_n$. This is because we assume that our predictive model will always get us in the neighbourhood of the true labels, and the utility of $SL$ is in helping distinguish between these points.

The combination of these 2 choices makes the learned $SL_{\phi_n}$ a “local” surrogate for $DL$, rather than a global one.

5 Experiments

We do a deep-dive using a task from Wilder et al. [14] to test the effectiveness of our approach.
5.1 Task Details

The aim of this task is to create predictions which help determine which websites to advertise on. The task is based on the Yahoo! Webscope Dataset [17] which contains the Click Through Rates (CTRs) for (a) \( M \) different websites, and (b) \( N \) different users (or demographic groups, more generally), for multiple advertisements. The matrix of CTRs per-advertisement comprises the set of predictions \( y \), where the rows correspond to websites and the columns correspond to users.

To simplify the prediction problem, the matrix is broken down row-wise into a set of vectors \([y^1, \ldots, y^M]\), each of which represent the CTRs for users on that website. Then, the set of features \( x_i \) for a given website is obtained by scrambling the CTRs of the corresponding row \( y_i \) using a random matrix of the same dimensionality that is multiplied by \( y_i \).

Finally, the optimization problem involves selecting the best \( B \) (budget) websites on which to advertise such that the expected number of users that click on the ad at least once is maximised. Mathematically, this is:

\[
\mathbf{z}^*(\hat{y}) = \arg \min_{\mathbf{z}} \frac{1}{N} \sum_{j=0}^{N} (1 - \prod_{i=0}^{M} (1 - z_i \cdot \hat{y}_{ij}))
\]

\[
s.t. \sum_{i=0}^{M} z_i \leq B \quad \text{for } i \in \{1, \ldots, m\}
\]

where \( \hat{y} \) is an \( M \times N \) matrix of the number of websites \( M \) by the number of users \( N \), \( B \) is the total budget, and \( \mathbf{z} \) is a vector of indicator variables that denotes whether a given website \( i \) is chosen \( z_i = 1 \) or not \( z_i = 0 \).

The requirement that \( z_i \in \{0, 1\} \) leads to zero-gradient issues (along the lines of the example in the introduction). As a result, the ‘multi-linear relaxation’ suggested in the paper is to remove this constraint and allow for fractional values. The interpretation, then, is that \( z^j \) denotes the probability of choosing website \( i \) such that, in expectation, only \( B \) websites are chosen. However, an important fact to note is that, while this relaxation may allow for non-zero gradients, the induced DL is non-convex because of the \( \prod_{i=0}^{M}(1 - z_i \cdot \hat{y}_{ij}) \) term in the objective.

**Note:** This problem is a maximization problem (rather than a minimization one that we’ve considered in the general formulation). While the formulation remains the same, the notion of decision loss is a bit of a misnomer because higher \( DL \) is better for maximisation problems. To reduce confusion, we instead use the term “Decision Quality” or \( DQ \) instead of \( DL \) from here on out.

5.2 Basic Results

We train a 3-layer feedforward neural network predictive model \( M_\theta \) to predict \( \hat{y} \) based on the learned surrogate loss functions \( SL_\phi \) and compare it to the following baselines:

1. Random: The predictions are sampled uniformly at random from \([0, 1]^{\dim(y)}\).
2. Optimal: The predictions are equal to the true labels \( y \).
3. MSE: \( M_\theta \) is trained on the standard MSE regression loss \( \frac{1}{N} \sum_{n=1}^{N} ||\hat{y}_n - y_n||^2 \).
4. DFL: \( M_\theta \) is trained directly on \( DQ \) using the end-to-end backpropagation strategy proposed by Wilder et al. [14].

The loss functions were learned with 500 samples and using the “All-Perturbed” sampling strategy. The results have been collated in Table 1.

There are a few things worth noting in these results:

1. **DFL can be very hit-or-miss:** Across the 10 problem instances, DFL gets either close to optimal (0.9+ normalised test decision loss on 5 instances, and \( \approx 0.75 \) on 2 others), or is close to random (\(< 0.15 \) normalised test DL on 5 instances). This suggests a sort of bi-modal distribution where DFL either works or doesn’t on certain problem instances. We hypothesise that this is due to
Table 1: A table mapping the loss function used to train $M_\theta$ to the corresponding model’s $DQ$ on test-data, re-scaled so that 0 corresponds to guessing at random and 1 corresponds to perfect predictive power. **Higher is better.**

| Approach          | Normalised $DQ$ On Test Data |
|-------------------|------------------------------|
| Absolute Baselines|                              |
| Random            | 0.000                        |
| Optimal           | 1.000                        |
| 2-Stage Baselines |                              |
| MSE               | 0.556 ± 0.197                |
| Decision-Focused Baseline |          |
| MSE               | 0.651 ± 0.386                |
| NN                | 0.154 ± 0.459                |
| Learned Loss      |                              |
| Weighted-MSE      | 0.564 ± 0.211                |
| Quadratic         | 0.962 ± 0.0290               |

1. **The non-convexity of the ‘relaxation-based’ surrogate used by DFL, which may lead to bad local optima.**
2. **Our ‘Quadratic’ SL consistently does well:** Unlike other methods in the table, the standard deviation for this approach is low (it gets close to the optimal for each of the 10 different problem instances).
3. **The choice of loss functions is important:** Just using a (vanilla) Neural Network or a weighted-version of MSE to learn SL does not lead to good outcomes.

### 5.3 Sanity Check

The experiment above shows that it’s possible to do just as well or better than “DFL” using a learned surrogate loss. However, a parallel question is whether training on $SL_\phi$ is leading to the same source of improvement (over MSE) as DFL, or whether they’re doing different things.

While we do not rigorously answer the question, in their paper Wilder et al. [14] hypothesise that the reason that DFL leads to better performance is because the $M_\theta$ learned using DFL more accurately models the sum of CTRs across users for a given website. Figure 1 (below) reproduces Figure 2 in Wilder et al. [14] and plots the true vs. predicted sum of CTRs.

![Figure 1](image)

**Figure 1:** A scatter plot of the predicted $\sum_j \hat{y}_{ij}$ (y-axis) vs. true $\sum_j y_{ij}$ (x-axis) sum of CTRs across users for different websites $i$. **The closer to the diagonal $y=x$, the better.**

As we can see, the model trained on DFL more accurately predicts this quantity. Similarly, we can see above that a model learned with our “Quadratic” surrogate loss also has this property, suggesting that it learns a similar form of relationship as DFL.

### 5.4 Ablations

One obvious question to ask is ‘How much are these results affected by the choices involved in learning $SL_\phi$?’ Towards address this question, we run 2 sets of experiments:

...
1. **Varying the sampling strategy used to learn SL:** In the table below, we compare the impact of different sampling strategies in learning \( SL_\phi \). To do this, we measure the quality of the models \( M_\theta \) learned when trained on \( SL_\phi \)s that were learned as a result of different sampling strategies:

| Approach       | Normalised Test \( DL \) (1-Perturbed) | Normalised Test \( DL \) (2-Perturbed) | Normalised Test \( DL \) (All-Perturbed) |
|----------------|----------------------------------------|----------------------------------------|----------------------------------------|
| NN             | −0.008 ± 0.584                         | 0.071 ± 0.389                          | 0.154 ± 0.459                          |
| Quadratic      | 0.393 ± 0.363                          | 0.428 ± 0.447                          | 0.962 ± 0.029                          |
| Weighted-MSE   | 0.709 ± 0.169                          | \textbf{0.780 ± 0.161}                 | 0.564 ± 0.211                          |

Table 2: Ablations across different sampling methods.

Based on the results above, it looks like the best sampling strategy is loss family-specific. While all of the NN-based models perform poorly, there is an improvement in the performance of Weighted-MSE when trained on "2-Perturbed" sampling.

2. **Varying the number of samples used to learn SL:** As above, we vary the number of samples used to learn \( SL_\phi \) and see the impact that it has on the performance of the model \( M_\theta \) that is trained on it.

| Approach       | Normalised Test \( DL \) (50 samples) | Normalised Test \( DL \) (500 samples) | Normalised Test \( DL \) (5000 samples) |
|----------------|---------------------------------------|----------------------------------------|----------------------------------------|
| NN             | 0.438 ± 0.207                         | 0.154 ± 0.459                          | 0.722 ± 0.236                          |
| Quadratic      | 0.393 ± 0.363                         | 0.962 ± 0.029                          | 0.996 ± 0.003                          |
| Weighted-MSE   | 0.765 ± 0.261                         | 0.564 ± 0.211                          | 0.863 ± 0.044                          |

Table 3: Ablations across different number of samples.

All of these models seem to perform best with the 5000 samples, with the results in boxes denoting ‘better performance that MSE’. Another positive is that the variance reduces as the number of samples increases (for Weighted-MSE and Quadratic), suggesting that better approximations of \( DL \) lead to more consistent outcomes.

### 5.5 Correlation between ‘quality’ of SL and decision quality

Now that we have a good sense of which approaches work, the next question that we’d like to answer is why. One obvious question is that, if \( SL \) is trying to model \( DL \), does how well \( SL \) does this correlate with its performance? We’ve seen above that, for a given loss family, increasing the number of samples (and as a result, the quality of the learned \( SL \)) improves outcomes. But how does this vary across different loss families?

To answer this question, we have to first quantify the notion of ‘how well \( SL \) models \( DL \)’. One way to do this is possibly to look at how well \( SL \) fits \( DL \) while learning \( SL \) from samples. If we look at the “(Sampled)” columns in Table, we find that there’s no correlation between the Test MAE (how good of an approximator \( SL \) is) and the normalised \( DL \) of \( M_\theta \) trained on \( SL \). In fact, the NN model has the lowest “Test MAE” but leads to the worst decision quality. One reason why \( SL \)’s Test MAE may not correlate with the performance of a model \( M_\theta \) trained on it is because we’re measuring the MAE on the set of Gaussian \( y^n \) points rather than the points which it actually encounters while training \( M_\theta \). For example, if \( y_n \) is not the minima of \( SL_{\phi_n} \) (for example for the NN-based \( SL \)), the predictions \( \hat{y}_n \) induced by \( SL \) might be quite far away from \( y_n \).

| Approach     | Train MAE (Sampled) | Test MAE (Sampled) | Test MAE (Real) | Normalised Decision Loss On Test Data |
|--------------|--------------------|-------------------|----------------|--------------------------------------|
| NN           | 0.0076 ± 0.0023    | 0.0076 ± 0.0023   | 0.0958 ± 0.0488 | 0.0882 ± 0.0893 | 0.154 ± 0.459 |
| Quadratic    | 0.0073 ± 0.0023    | 0.0085 ± 0.0026   | 0.0023 ± 0.0008 | 0.0098 ± 0.0008 | 0.962 ± 0.029 |
| Weighted-MSE | 0.0081 ± 0.0025    | 0.0081 ± 0.0025   | 0.0540 ± 0.0207 | 0.0524 ± 0.0382 | 0.364 ± 0.211 |

Table 4: A table showing the relationship between the quality of the learned loss for different classes of surrogate losses, and the performance of a model trained on said loss.
To account for this discrepancy, we also look at the MAE between $SL$ and $DL$ for the $\hat{y}$ points predicted by the optimal $M_\theta$ (trained on $SL$) on the train and test dataset. The results can be found under the "(Real)" columns in Table 4. Here, we see that there is a correlation between Train MAE (how close $SL$ was to $DL$ while training $M_\theta$) and the performance of the $M_\theta$ trained using $SL$.

Moreover, this error also seems to be strongly predictive of how well the learned model does. Specifically, the mean absolute $DL$ on test data if $M_\theta$ made optimal predictions is $\approx 0.2$, whereas the mean $DL$ is $\approx 0.087$ if $M_\theta$ makes random predictions. Then, for example, Weighted-MSE has a Test MAE of $0.147$. This is equal to a normalised $DL$ of $0.147 - 0.087 \approx 0.53$ which is close to what we actually observe in the experiments.

6 Limitations and Open Questions

Despite the strong results in the experiments above, there are potential caveats which represent directions for future work:

1. **The dimensionality of $y$ will be a challenge:** Because $SL_\phi$ is a $\text{dim}(y)$-dimensional function, if $y$ is high-dimensional, it will be difficult to learn a good surrogate loss. To address this while learning $M_\theta$, one typically makes the assumption that all the dimensions in $y$ are independent, but this trick isn’t something we can extend to learning $SL$ because it has to incorporate information about how important different prediction components are in relation to each other. As a result, it seems like our approach is particularly well-suited to problems in which $\text{dim}(y)$ is low, but running the optimization involved in $DL(\hat{y}, y)$ is expensive.

   One way to get around this issue is to learn a model that is independent of $\text{dim}(y)$, for example by learning a function that predicts the entries $H_{ij}$ of the matrix corresponding to our “Quadratic” $SL$. However, we leave this for future work.

2. **Our localness assumptions may be violated for some classes of problems:** There may be cases in which it’s impossible to make predictions that are “close to the true labels $y$”. For example, if $y \in \{0, 1\}^{\text{dim}(y)}$ or there’s large “label noise”, no predictive model can get arbitrarily close to the true labels. As a result, the Taylor approximation that’s central to the success of our Quadratic $SL$ may not be applicable.

7 Conclusion

We provide a generalizable approach that learns faithful task-specific convex surrogate loss functions for predict-then-optimize problems. In the experiments, we find that our approach performs better even than the (non-convex) handcrafted surrogate for our chosen problem, despite having no task-specific structure to aid it. We are currently working on extending our approach to more domains to highlight its generalizability.

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