ROBUST LOSSES FOR DECISION-FOCUSED LEARNING

A PREPRINT

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ABSTRACT

Optimization models used to make discrete decisions often contain uncertain parameters that are context-dependent and are estimated through prediction. To account for the quality of the decision made based on the prediction, decision-focused learning (end-to-end predict-then-optimize) aims at training the predictive model to minimize regret, i.e., the loss incurred by making a suboptimal decision. Despite the challenge of this loss function being possibly non-convex and in general non-differentiable, effective gradient-based learning approaches have been proposed to minimize the expected loss, using the empirical loss as a surrogate. However, empirical regret can be an ineffective surrogate because the uncertainty in the optimization model makes the empirical regret unequal to the expected regret in expectation. To illustrate the impact of this inequality, we evaluate the effect of aleatoric and epistemic uncertainty on the accuracy of empirical regret as a surrogate. Next, we propose three robust loss functions that more closely approximate expected regret. Experimental results show that training two state-of-the-art decision-focused learning approaches using robust regret losses improves test-sample empirical regret in general while keeping computational time equivalent relative to the number of training epochs.

1 Introduction

Real-world optimization problems, often formulated and solved as mixed-integer linear problems (MIPs) – such as shortest path problems or machine scheduling problems – involve parameters whose value is not known exactly. It is natural to use data to predict the uncertain parameters' values based on contextual information.

In predictive (regression) problems the goal is to make the most accurate prediction possible in the sense of prediction error. However, since there remains uncertainty around the predictions, and their purpose is to more accurately solve a downstream optimization problem, such a measure of prediction accuracy is of little relevance: the quality of the resulting decisions is what is important. This is the main premise of *decision-focused learning* (DFL) (also named predict+optimize or smart/end-to-end predict-then-optimize), and contrasts with 2-stage learning that is focused on prediction accuracy. DFL was first pioneered specifically for portfolio selection based on financial time series by Bengio [1997], and more generally introduced by Elmachtoub and Grigas [2022].

Learning based on decision errors obtained through solving a MIP faces difficulty, since the gradient of the decisions relative to the predicted parameters is zero almost everywhere and otherwise undefined [Vlastelica et al., 2019]. Because of this, approximation methods have been introduced and shown to be more effective than 2-stage learning [Elmachtoub and Grigas, 2022, Berthet et al., 2020]. The loss used in these methods is based on *empirical regret*, i.e., the loss incurred from not making the optimal decision for a given, empirical scenario. However, we observe that in expectation this empirical regret deviates from the expected regret as it underestimates the probabilistic nature of expected regret, i.e., might lead to a form overfitting on the empirical sample.

Recognizing this shortcoming in loss functions in DFL, this paper develops three contributions to the literature:

1. We examine the usage of empirical regret from an uncertainty perspective, showing how empirical regret can lead to poor generalization and biased learning towards uncertain parameters with high variance.

- 2. We propose three different robust loss functions that simultaneously (1) improve conditional mean estimation, (2) are robust against errors in the mean estimation, and (3) do not increase computational expense relative to the number of training epochs.
- We study two state-of-the-art DFL methods using the proposed robust losses compared to them using empirical regret. On three experimental problems average test-sample empirical regret is improved without additional overhead.

2 **Problem Formulation**

In this work we adopt the problem setting as introduced in Elmachtoub and Grigas [2022]. Observing some contextual information in the form of feature values $z \in \mathbb{R}^m$, the goal of the decision maker is to solve the following stochastic optimization problem with linear objective:

$$\min_{x \in X} \mathbb{E}_{c \sim \mathcal{C}_z}[c^T x | z],\tag{1}$$

where X denotes the set of feasible decisions and C_z is the conditional distribution of uncertain objective coefficients $c \in \mathbb{R}^n$ given feature values z. Since C_z is unknown, training a parametric predictor $f_{\theta}(z)$ can assist in picking good decisions. Ideally we find a predictor s.t. for each z we make a decision that has an equal objective to (1), i.e.,

$$\mathbb{E}_{c \sim \mathcal{C}_z}[c|z]^T \left[\operatorname*{argmin}_{x \in X} f_{\theta}(z)^T x \right] = \min_{x \in X} \mathbb{E}_{c \sim \mathcal{C}_z}[c^T x | z]$$

When the prediction problem is seen as separate from the optimization problem, regression is performed with coefficients c as responses to features z by minimizing prediction error. We will refer to this as 2-stage learning. However, since the decision maker's goal is not to make accurate predictions but to make optimal decisions, it is preferable to minimize decision error, which is the main premise of DFL. To attain this goal, Elmachtoub and Grigas [2022] introduce a loss function based on the notion of *regret*, i.e., the loss incurred by not making the optimal decision given z:

$$l_{\rm emp}(\hat{c}, c) = c^T x^*(\hat{c}) - c^T x^*(c), \tag{2}$$

where $\hat{c} = f_{\theta}(z)$, and $x^*(c) = \operatorname{argmin}_{x \in X} c^T x$ is the optimal decision when c are the objective coefficients. We will refer to this as *empirical regret*, as it is the regret in an empirical realization of (z, c). This loss is a natural choice, for when (z, c) is realized the loss is equal to 0 when the empirical optimal decision is made.

In practice, however, a loss of 0 is unachievable as c is a sample realization of probability distribution C_z . This becomes more apparent when looking at what happens when we try to learn a predictive model using the empirical regret loss. When minimizing any empirical loss through a method like gradient descent, we are effectively minimizing a surrogate of the true expected loss. Indeed, given the empirical regret loss, the expected loss we are minimizing is

$$\mathbb{E}_{c \sim \mathcal{C}_z}[l_{emp}(\hat{c}, c)] = \mathbb{E}_{c \sim \mathcal{C}_z}[c^T x^*(\hat{c})|z] - \mathbb{E}_{c \sim \mathcal{C}_z}[\min_{x \in X} c^T x|z]$$
$$= \mathbb{E}_{c \sim \mathcal{C}_z}[c|z]^T x^*(\hat{c}) - \mathbb{E}_{c \sim \mathcal{C}_z}[\min_{x \in X} c^T x|z]$$

with the outer expectation $\mathbb{E}_{z}[\cdot]$ omitted for clarity.

The first term in this expression is equal to the gained objective when choosing $x^*(\hat{c})$; however the second term is in general not equal to the gained objective when making the optimal decision as defined in (1), since the expectation and minimization are not interchangeable and thus

$$\mathbb{E}_{c \sim \mathcal{C}_z}[\min_{x \in X} c^T x | z] \le \min_{x \in X} \mathbb{E}_{c \sim \mathcal{C}_z}[c^T x | z].$$
(3)

Despite this term being independent of the predictive model, it can cause the loss to be positive when an expected optimal decision is being made. Because of this it would be natural to desire a loss in which the decision error is relative to the exact underlying optimization problem:

$$l_{\mathbb{E}}(\hat{c}, \mathcal{C}_z) = \mathbb{E}_{c \sim \mathcal{C}_z}[c|z]^T x^*(\hat{c}) - \min_{x \in X} \mathbb{E}_{c \sim \mathcal{C}_z}[c^T x|z].$$
(4)

Since in practice data is often only available in the form of realized value pairs $D = \{(z_i, c_i) : i \in \{1, ..., t\}\}$, this loss (4) cannot be obtained empirically, which makes it necessary to have an effective surrogate. In this paper, we aim to understand the impact of using empirical regret as a surrogate and propose alternatives to mitigate its shortcomings. We



Figure 1: Observed coefficients c (profit) per feature value z (temperature) and optimal linear predictors $f_{\theta}^*(z)$ according to different loss functions. The example problem is a coffee stand owner deciding what treat to make from their daily batch of chocolate. There are 3 possible weather related decisions X: chocolate ice cream \blacklozenge , chocolate cookies \blacksquare or hot chocolate \blacksquare . The linear predictors are the lines with corresponding colour and shade. The shaded area \blacksquare is considered to be sub-optimal.

begin by showing what issues can arise when training using empirical regret. The main intuition is the following: When using empirical regret, training is biased towards empirical optimal decisions that are not necessarily expected optimal decisions. This is due to a form of overfitting, i.e., uncertainty causing a mismatch between training and test data, and the non-smoothness of a discrete optimization problem, which can cause significant changes in optimal decisions by only small perturbations. To analyze the impact of uncertainty more formally, we make the distinction between epistemic and aleatoric [Kiureghian and Ditlevsen, 2009]. Epistemic uncertainty is uncertainty that occurs due to a lack of knowledge, which in practice often equates to not having enough representative data available. Aleatoric uncertainty is the uncertainty inherent to some underlying process and is therefore irreducible. In our DFL setting, we assume there exists a distribution C_z for every z that contains purely aleatoric uncertainty, but since we are limited by finite data the distributions C_z are unknown to us – the epistemic uncertainty.

Impact of epistemic uncertainty Epistemic uncertainty makes generalization challenging as there is no complete knowledge, hence making it impossible to exactly learn the underlying process. This general challenge for predictive problems is exemplified in DFL due to the focus on optimal decisions. When using 2-stage learning, the predictive model is trained to predict all coefficients as accurate as possible. When using DFL with empirical regret, the focus is on predicting the objective coefficients related to optimal decisions, i.e., objective coefficients that directly impact the empirically optimal decisions' objectives. This is because empirical regret (2) is defined as the difference of the obtained objective given prediction \hat{c} and the empirically optimal objective. This means that empirical regret disregards objective coefficients that are not related to optimal decisions.

Figure 1 gives an illustrative example in which 2-stage learning using the mean squared error and DFL using empirical regret both lead to likely sub-optimal predictors. Note that in Figure 1c, the linear predictors are empirically optimal as long as \blacksquare is predicted with low values of z and \blacklozenge with high values of z, which makes the linear predictor of \blacksquare optimal as long as it does not predict the highest value for any of the realized points (c, z). This means the predictors denoted in Figure 1b are also optimal according to empirical regret, but it has such a wide range of parameter values that are considered optimal it is likely to predict low values for z. The shaded sub-optimal considered area is determined assuming a linear interpolation between the observed points closest to the middle equals the expected value of c.

Impact of aleatoric uncertainty In general, a lack of enough representative data leads to epistemic uncertainty. However, even when there is plenty of representative data and only aleatoric uncertainty, we observe that using the empirical loss biases learning towards objective coefficients that have high variance, with variance being a measure of aleatoric uncertainty. This is because the predictive model parameters that affect high variance objective coefficient predictions \hat{c} are more likely to be updated during training than those that affect low variance objective coefficient predictions \hat{c} . This can be problematic because it can make predictions of low variance objective coefficients less accurate (also with respect to decision quality), while it is these objective coefficients that relate to optimal decisions with a less uncertain objective value.

To provide intuition behind this observation, we first note that the empirical regret loss is a measure that is dependent on two decisions, i.e., the empirical optimal decision $x^*(c)$ and the predicted optimal decision $x^*(\hat{c})$. This means that a

true gradient would adjust only objective coefficients that relate to these decisions' objective values. This means that if certain coefficients are more likely to be related to optimal decisions' objective values, they are more likely to be updated during training. We provide an example to show that the variance of objective coefficient affects this.

Example 1. Consider optimization problem (1), where decision set X is finite and each decision has its own objective coefficient, i.e., $X = \{x : x \in \{0,1\}^n, \sum_{i=1}^n x_i = 1\}$, where we recall that $c \in \mathbb{R}^n$. Assume that all c_i are independent and have $\mathbb{E}_{c \sim C_z}[c_i|z] = 0$ but different variance. In expectation, all decisions have equal objective value 0. However, empirically we observe the decision with the lowest realized coefficient as optimal. If a decision x_i has a coefficient with $Var(c_i) = 0$, it is only optimal if all other coefficients are realized greater or equal to 0. If x_i has a coefficient with high variance, it is more likely to be optimal as its coefficient is more likely to realize the lowest value. Considering a dataset with realized values, decisions with higher variance coefficients are more often empirically optimal.

A formal proof is provided in Appendix A.

3 Robust Losses

We introduce novel DFL losses with the goal to mitigate the issues of poor generalization and biased learning that can arise when using empirical regret as a loss. We show that these issues can be mitigated by finding an estimator of $\mathbb{E}_{c\sim C_z}[c|z]$ with lower variance than c and making the loss robust against the estimation error. Based on this we define three novel loss functions.

First, we reiterate that the predictor f(z) = c would lead to an empirical regret loss of 0 that is unattainable due to C_z being the underlying distribution given z. A perfect predictor would be $f(z) = \mathbb{E}_{c \sim C_z}[c|z]$, which is because of the assumption of the uncertain parameters c being linear in the objective function, as

$$\min_{x \in X} \mathbb{E}_{c \sim \mathcal{C}_z}[c^T x | z] = \min_{x \in X} \mathbb{E}_{c \sim \mathcal{C}_z}[c | z]^T x$$

leads to an expected regret loss of 0. This is important as it shows that a scalar valued predictor can be expressive enough and we do not need to be able to predict the whole distribution C_z to have a strong predictor. This also means that we can still consider the deterministic problem $x^*(f(z))$ as the problem the decision maker solves when observing feature values z in practice. This consideration is important in designing the robust losses we propose, as this means that during training we can still evaluate the loss by solving a deterministic problem without potentially losing performance. Since DFL using gradient descent is already relatively computationally expensive due to frequently having to solve an optimization problem, it is important computation time is not increased further Mulamba et al. [2020].

To find a good surrogate for the expected regret loss, we first look at the empirical regret as surrogate. When we optimize using empirical regret, effectively the realized c are used as an estimate of $\mathbb{E}_{c\sim C_z}[c|z]$ when considering the expected regret as the true regret. Since the realized c is a sample realization from C_z , the expected estimation error is equal to the variance of C_z . This means that the empirical optimal decision $x^*(c)$ can be significantly different from the expected optimal decision $x^*(\mathbb{E}_{c\sim C_z}[c|z])$, which leads us to two main principles in designing the robust losses:

- 1. Determine an estimator of $\mathbb{E}_{c \sim C_z}[c|z]$ that has lower variance than c.
- 2. Determine an approach to find optimal decisions that are robust against the estimation error of $\mathbb{E}_{c \sim C_z}[c|z]$.

We introduce two losses based on the second principle, followed by a loss based on the first principle that naturally extends to a generalization that also includes the second principle. Figure 2 visualizes the three proposed losses compared to empirical regret.

3.1 Robust optimization (RO) loss

Assuming c is an erroneous estimation of $\mathbb{E}_{c \sim C_z}[c|z]$, we consider empirical optimal decision $x^*(c)$ as an erroneous optimal decision. Instead of using $x^*(c)$, we can use the decision that minimizes the worst-case value of this error given some assumptions, i.e., robust optimal decision

$$x_{\text{RO}}^*(c) = \min_{x \in X} \max_{c \in U_c} c^T x,$$
(5)

where U_c is an *uncertainty set*, i.e., a set that specifies the possible estimation error of c. This formulation is commonly used in Robust Optimization (RO), where the goal is to find decisions that are optimal given the worst case in some specified uncertainty set Bertsimas et al. [2011].

Since in RO the retrieved optimal decision is robust against the uncertainty specified by the uncertainty set, a proper specification of the latter is important. An uncertainty set that is too small makes the optimal decision not robust against



Figure 2: Visualization of robust DFL losses compared to the empirical regret loss (full predictive pipeline is only displayed on the left). The robust losses are constructed through using an optimization model (optimizer) that is robust against the mean estimation error and/or using a different mean estimator than empirically observed c. From left to right: empirical regret (l_{emp}), RO loss (l_{RO}), top-k loss (l_{top-k}), k-NN loss (l_{k-NN}).

the actual uncertainty, while an uncertainty set that is too large leads to conservative decisions that could be far from expected optimal. Further, depending on the uncertainty set the optimization problem (5) has a tractable reformulation. We propose the RO loss defined as follows:

$$l_{\rm RO}(\hat{c}, c) = c^T (x^*(\hat{c}) - x^*_{RO}(c))$$

As a choice of uncertainty set we propose the *budget uncertainty set*, which is a special case of a polyhedron uncertainty set Bertsimas and den Hertog [2022]. This set is practical as it is not too conservative while it allows for a tractable reformulation of linear optimization problems, i.e., if the optimization problem has a linear objective and only linear constraints specifying the decision set X the reformulation does not increase complexity. Our setting is not limited to this model class, but having a linear tractable reformulation is helpful as it does not change the class of the problem: the budget uncertainty set reformulation of the MIPs we consider is a MIP. Since the robust formulation adds constraints and auxiliary decision variables, the problem can become harder (albeit also easier) to solve. However this is highly dependent on the problem and is not straightforward to quantify.

The budget uncertainty set allows us to model the estimation error of c as a percentage deviation ζ . We limit the individual coefficient percentage deviation and the total percentage deviation by ρ and Γ respectively, giving

$$U_{c} = \{ c \circ (1+\zeta) : ||\zeta||_{\infty} \le \rho, ||\zeta||_{1} \le \Gamma \},\$$

where \circ denotes the Hammard product. Depending on knowledge of the optimization problem and/or the uncertainty around *c* the uncertainty set can be adjusted. Our goal here is to show a proof of concept, leaving for the future a full exploration of specifying uncertainty sets in a DFL setting.

3.2 Best k decisions (top-k) loss

An alternative to finding a decision that is robust against erroneous estimations is to consider multiple decisions that are close-to optimal. For instance, suppose that in the example in Figure 1 the second-best decision is also considered as optimal, then its coefficients would not be disregarded. Looking at multiple close-to optimal decisions can lead to a good area in the decision space, compared to a single optimal decision that might lay in a narrow global optimum. Moreover, high variance of c as an estimate of $\mathbb{E}_{c\sim C_z}[c|z]$ can lead to significantly different decisions, while considering multiple close-to optimal decisions can lead to certain decisions being found more often and therefore a more stable signal.

The process of finding multiple quality decisions is not complicated. Independent of the method that is used for finding an optimal decision, this method can be used subsequently while excluding already found decisions. This makes the loss we propose viable, as we propose a loss that evaluates regret against the best k decisions (top-k):

$$l_{\text{top-}k}(\hat{c},c) = \frac{1}{k} \sum_{j=1}^{k} c^{T}(x^{*}(\hat{c}) - x^{*}_{(j)}(c)),$$

where $x_{(j)}^*(c) := \operatorname{argmin}_{x \in X \setminus \{x_{(1)}^*(c), \dots, x_{(j-1)}^*(c)\}} \{c^T x\}.$

Alternatively one could consider not specifying the number of decisions that is considered as good enough, but specifying a certain quality metric like a certain percentage from the optimal objective. This would depend on the use-case and will not be considered here.

3.3 k-nearest neighbour (k-NN) loss

An estimator of $\mathbb{E}_{c\sim C_z}[c|z]$ that has lower variance than c has to utilize the training data, while preferably being unbiased and consistent. This makes k-nearest neighbour (k-NN) regression a strong candidate as it is a non-parametric regression that has extensively studied strong asymptotic uniform consistency results [Cheng, 1984] and more recently also finite-sample uniform consistency results [Jiang, 2019]. Being non-parametric is beneficial as we will train a parameterized predictive model using signals from the estimator. If the estimator would be in the same model class, this would potentially amplify predictive and decision errors due to model misspecification. The k-NN estimator given feature values z is defined as the arithmetic mean of $c_{(j)}$ where

$$(z_{(j)}, c_{(j)}) = \operatorname*{argmin}_{(z', c') \in D \setminus \bigcup_{i=1}^{j-1} \{(z_{(i)}, c_{(i)})\}} ||z' - z||$$

is the *j*-th closest data point in the feature space, $|| \cdot ||$ is some norm (we use the Euclidean norm) and *D* the set of data points. The consistency of the *k*-NN estimator is intuitive, as with an increasing number of data realizations, the *k* nearest neighbours converge in distance, i.e.,

$$||z_{(j)} - z|| < \epsilon \quad \forall j \in \{1, \dots, k\}.$$

If the distance between feature values goes to zero, the conditional probability distributions $C_{z_{(j)}} \forall j \in \{1, ..., k\}$ converge to C_z as well, assuming the underlying cumulative distribution function is continuous in z. This means that when the number of data realizations goes to infinity, the realized coefficient values $c_{(1)}, \ldots, c_{(k)}$ are samples drawn from the same distribution C_z . Taking the mean of this is then a sample mean and therefore a consistent estimator of $\mathbb{E}_{c\sim C_z}[c]z]$ with variance $\operatorname{Var}_{c\sim C_z}(c)/k$.

These consistency results do not extend to the decision space, as optimization problem $x^*(\cdot)$ is a discontinuous multivalued function. Despite this, we can expand on the reasoning above: If the k nearest neighbours are somewhat representative of a set of samples from conditional probability distributions C_z , the obtained decisions $x^*(c_{(1)}), \ldots, x^*(c_{(k)})$ could all be empirical optimal decisions given z. Since our k-NN estimator will still have some estimation error, we consider multiple potential optimal decisions in a similar fashion as in designing the top-k loss. This way we naturally include the second principle we proposed for designing robust losses. The loss we propose is the average over the empirical regret of k nearest neighbours:

$$l_{k-NN}(\hat{c},c) = \frac{1}{k} \sum_{j=1}^{k} c_{(j)}^{w}{}^{T}(x^{*}(\hat{c}) - x^{*}(c_{(j)}^{w})),$$

where the values of the neighbours are adjusted based on some interpolation weight $w \in [0, 1]$:

$$c_{(j)}^{w} = wc_{(j)} + (1 - w)c_{(j)}$$

We introduce this interpolation weight to make sure the k-NN estimator and therefore loss function remains distinct for all observations (z, c). Without this weight, multiple different observations can have the same k nearest neighbours and therefore the same estimator. This is not a general problem in k-NN regression, but it arises because we use the estimator in-sample, i.e., we provide an estimate of observations c that have a known realized value. This problem arises especially when there is little data available as it leads to over-simplification of the existing relationships, i.e., increased assumption bias. This makes w a tool to find a sweet spot in the bias-variance trade-off [Geman et al., 1992]. In the same work, the k-NN estimator is considered as an example where increasing k increases bias, while decreasing k increases variance. Due to our in-sample usage of the k-NN estimator, varying k does not solve the issue of different observations having equal estimators. We note that w = 0 makes the k-NN loss equal to the empirical regret loss and therefore this loss is more general.

3.4 Computational Considerations

Training a predictive model using gradient-based approaches requires frequently evaluating (solving) optimization problem $x^*(\cdot)$. In every epoch, $x^*(f_{\theta}(z))$ needs to be evaluated for each data point (z, c) to obtain the loss and/or

gradient. This is the most computationally expensive part of training and we will therefore quantify the computational expense in a number of problem evaluations. Looking at the empirical regret loss, $x^*(c)$ does not change during training, and can therefore be precomputed. Given t data points and s epochs, problem $x^*(\cdot)$ is solved t * (s + 1) times.

The proposed robust losses increase precomputation time i.e., computation time before the training, but do not increase training time per epoch. For the k-NN and top-k loss the total number of evaluations is t * (k + s). In practice s is significantly larger than k and therefore the increase in total time is small. For the RO loss, the same number of evaluations is done compared to the empirical regret loss. While it could be that solving the robust problem formulation takes longer, this is also during precomputation at most t times.

Below we apply our losses to two state-of-the-art gradient-approximation approaches, Smart "Predict, then Optimize" (SPO+) of Elmachtoub and Grigas [2022] and the Perturbed Fenchel–Young Loss (PFYL) of Berthet et al. [2020]. Since they are approximations, it is not given that above analysis on problem evaluation equates to the same for the approximate gradients. In Appendix B we show that the robust losses are readily applied to these approaches.

4 Experimental Evaluation

We compare SPO+ and PFYL (number of samples M = 1, perturbation amplitude $\sigma = 1$) trained using empirical regret as loss to the same approaches using the presented robust losses (RO, top-k, k-NN), with 2-stage learning using mean squared error as an additional baseline. All predictive models are linear models. We use Python-based open-source package *PyEPO* Tang and Khalil [2022] for the data generation of two experimental problems and the training, where the robust losses are implemented on top of the existing code. We use *Gurobi* version 10 Gurobi Optimization, LLC [2021] as the optimization problem solver. We compare the results on three experimental problems: shortest path, travelling salesperson, and energy-cost aware scheduling.

For simplicity, we do not tune the hyperparameters of the robust losses, but use the same value for all problem configurations. For the top-k loss we use k = 10; the same for the k-NN loss where w = 0.5. For the RO loss we set $\rho = 0.5$ and $\Gamma = \frac{n}{8}$, where n = |c|. The batch size is 32.

4.1 Experimental Problems

Shortest path & travelling salesperson The shortest path problem considers a decision maker that has as goal to find the shortest path from start (NW) to end (SE) over a pre-specified grid (10 × 10) with uncertain costs (objective coefficients), allowing only viable paths modelled by a vector of binary decision variables. The travelling salesperson problem also aims at finding a shortest path, but instead of a grid there is a set of fully connected nodes (20) that all need to be visited. For both problems data is generated as in PyEPO Tang and Khalil [2022], with feature vectors z of size 5 and the polynomial degree parameter fixed at 6. We look at different noise half-width values $\bar{\epsilon} \in \{0, 0.5, 1\}$ that multiply the generated objective coefficients by $\epsilon \sim U(1 - \bar{\epsilon}, 1 + \bar{\epsilon})$, and different training set sizes $t \in \{100, 1000\}$. We consider these parameter values to mimic different levels of aleatoric and epistemic uncertainty. The noise multiplies the existing data generating distribution by another distribution that increases variance and therefore aleatoric uncertainty, while the training set size is a measure of how much knowledge we have and therefore mimics epistemic uncertainty. In all cases a validation and test set of size 100 and 1000 are used respectively. 200 epochs are run for t = 100, and 100 epochs for t = 1000. Since the data generation is a random process, we run 20 generated datasets to be able to measure significance.

Energy-cost aware scheduling As a third experimental problem we look at energy-cost aware scheduling Simonis et al. [1999] as done before in a DFL setting Mandi et al. [2022]. The dataset consist of historical Irish energy price data at 30-minute intervals from 2011-2013, including 789 days Ifrim et al. [2012]. The optimization problem consists of scheduling a given number of tasks (3) on a given number of machines (10) with a certain resource capacity. Each task has a given energy consumption per hour and the goal is to minimize the total daily energy consumption. Energy prices are uncertain however and are therefore predicted. Instead of using the features in the dataset, we consider the predictive problem as a time series problem consisting of predicting the next day using the day before, both consisting of 48 values. This way the uncertain objective coefficients share the same feature vector as defined in problem formulation (1). We also add noise to the data and we use training sizes of $t \in \{100, 500\}$ with a validation and test set of 100 each. Given we have 789 days, we create 5 non-overlapping data partitions of the data preserving time order when t = 100. When t = 500 we use a single partition, and in both cases we omit the last 89 days. We run 50 epochs for every training run.

Further details on the experimental problems are provided in Appendix C.



Figure 3: Test set mean normalized empirical regret in % (y-axes) on 3 experimental problems with different noise $(\bar{\epsilon})$ and training size (t) values. Approaches are denoted by patterns; used losses by colour (mean squared error is used for 2-stage). Error bars denote one in-sample standard deviation on both sides of the mean. Mean values of robust losses that are significantly different (paired t-test, $\alpha = 0.05$) from their empirical regret counterpart are denoted with * (better) or × (worse). A tabular version of the results is shown in Appendix D.

4.2 Results

Figure 3 shows all results. For the shortest path and travelling salesperson, we see that when t = 100 in 24 out of the 36 comparisons the robust loss performs significantly better and it never performs significantly worse compared to the empirical loss. When t = 1000, we see 13 significantly better and 4 significantly worse results, out of which 3 are on the shortest path problem with $\bar{\epsilon} = 0.0$. From this we conclude that all robust losses are effective when data is limited, while particularly the k-NN loss is effective when there is plenty data. Due to the limited size of the dataset, we see only 2 significant results for the energy-cost aware scheduling problem. We do note however that these are both in favour of the robust loss and in all other configurations a robust loss also performs best.

5 Discussion and Related Work

In this paper the proposed losses are evaluated on DFL gradient-approximation approaches Elmachtoub and Grigas [2022], Berthet et al. [2020], where we assume the uncertain parameters are coefficients linear in the objective. These approaches are effective since exact gradient methods using the Karush-Kuhn-Tucker conditions in general require a quadratic program as the inner optimization problem to have defined non-zero gradients Amos and Kolter [2017]. This can be extended to linear programs by adding a quadratic Wilder et al. [2019] or log-barrier Mandi and Guns [2020] objective term. For MIPs, Ferber et al. [2020] introduce a cutting-plane approach to convert the discrete problem into an equivalent continuous problem, which is computationally expensive and therefore less applicable compared to gradient-approximation approaches.

Gradient-approximation approaches have so far not been able to directly deal with a non-linear objective function or uncertain parameters in the constraints, but Silvestri et al. [2023] introduced score function gradient estimation for DFL, by predicting a distribution instead of a point. Extending our work to this setting will be interesting.

Empirical regret is in general used as a loss in DFL and therefore studied here, but some alternative losses have been proposed. Mulamba et al. [2020] introduce a contrastive loss that uses non-optimal decisions as negative samples to attain more effective gradients. Mandi et al. [2022] extend on this work by defining DFL as a learning-to-rank problem, i.e., accurately ranking decisions leads to being able to pick the optimal decisions. Losses in these two works are especially effective in reducing training time for comparable decision quality. Shah et al. [2022] propose an approach to learn losses that are convex and therefore practical for training, however these losses are learned based on empirical regret.

Sadana et al. [2023] provide a recent survey of predict-then-optimize approaches, also discussing non end-to-end approaches that take uncertainty into account with respect to the optimization problem and in that sense share similarities with our work. For example, Sun et al. [2023] explicitly model the uncertainty in the predictive model by calibrating it to the optimization model objective without training end-to-end.

Since we show that our proposed robust losses improve generalization when training data is limited, a natural alternative would be applying regularization, as effectively used in deep learning Kukačka et al. [2017]. Elmachtoub and Grigas [2022] use a mean squared error or a mean absolute error term for regularization. This allows for improving prediction accuracy while preserving decision quality Tang and Khalil [2022], but it does not improve decision quality which we do observe using robust losses.

6 Conclusion

Decision-focused learning is gaining considerable recent interest due to its effective end-to-end approach to data-driven optimization. This paper investigated the shortcomings of using empirical regret in DFL, and proposed a trio of robust loss functions to mitigate the issues of poor generalization and biased learning. Experimental results show improved test-sample empirical regret without inflating computational time. Future work includes studying RO uncertainty sets and fine-tuning hyperparameters of the proposed losses.

7 Acknowledgements

This project has received funding from the EU Horizon 2020 programme under grant number 964505 (Epistemic AI).

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Appendix

A Formal proof impact variance example

In Example 1, we show that DFL with empirical regret can be biased towards high variance objective coefficients. This example is aimed at providing intuition and therefore does not contain a formal proof. Below we provide this proof.

Recall the decision maker's optimization problem:

$$\min_{x \in X} \mathbb{E}_{c \sim \mathcal{C}_z}[c^T x | z],$$

where X denotes the set of feasible decisions and C_z is the conditional distribution of uncertain objective coefficients $c \in \mathbb{R}^n$ given feature values z. Now we make the same assumptions as in the example, where (with abuse of notation) $c_i \in c, i \in \{1, ..., n\}$ have some probability density function $c_i \sim f_i(x)$ and joint probability density function $c_i, c_j \sim f_{i,j}(x, y)$.

Assumption 1. Decision set X is finite and each decision has its own objective coefficient, i.e., $X = \{x : x \in \{0,1\}^n, \sum_{i=1}^n x_i = 1\}$.

Assumption 2. Assume that $c_i \in c, i \in \{1, ..., n\}$ have a symmetrical probability distribution, i.e., $\forall i, \exists \bar{x}: f_i(\bar{x}+\delta) = f_i(\bar{x}-\delta) \ \forall \delta \in \mathbb{R}$.

Assumption 3. Assume that $c_i \in c, i \in \{1, ..., n\}$ are independent, i.e., $f_{i,j}(x, y) = f_i(x)f_j(y), \forall x, y$.

Assumption 4. Assume that $c_i \in c, i \in \{1, ..., n\}$ have an expectation of zero, i.e., $\mathbb{E}_{c \sim C_z}[c_i|z] = 0$, $\forall i$. (Note that under Assumption 2 $\mathbb{E}_{c \sim C_z}[c_i|z] = \bar{x}$.)

Assumption 5. There exist n_h decisions $X_h \subset X$ with coefficients with (high) variance $Var(c^T x_h) = \sigma_h^2$ and n_l decisions $X_l \subset X$ with coefficients with (low) variance $Var(c^T x_l) = \sigma_l^2$, where $n_l + n_h = |X|$.

Theorem 1. Assume |X| > 2. Given some z, we have that $\forall x_h \in X_h, x_l \in X_l$:

$$\mathbb{P}(x_h = x^*) > \mathbb{P}(x_l = x^*),$$

when $\lim_{\sigma_l^2 \to 0}$, where $x^* = \operatorname{argmin}_{x \in X} \mathbb{E}_{c \sim C_z}[c|z]$.

Proof.

$$\begin{split} \lim_{\sigma_{l}^{2} \to 0} \mathbb{P}(x_{l} = x^{*}) \\ & \stackrel{\text{a.s.}}{=} \mathbb{P}(x_{l} = x^{*}; c^{T}x_{l} = \mathbb{E}_{c \sim \mathcal{C}_{z}}[c^{T}x_{l}|z], \forall x_{l} \in X_{l}) \\ & \stackrel{(4)}{=} \mathbb{P}(x_{l} = x^{*}; \min_{x \in x} \mathbb{E}_{c \sim \mathcal{C}_{z}}[c^{T}x|z] = 0) \\ & = \mathbb{P}(x_{l} = x^{*}|c^{T}x_{h} > 0, \forall x_{h} \in X_{h})\mathbb{P}(c^{T}x_{h} > 0, \forall x_{h} \in X_{h}) \\ & \stackrel{(2,3)}{=} \frac{1}{n_{l}}(\frac{1}{2})^{n_{h}}, \\ & \lim_{\sigma_{l}^{2} \to 0} \mathbb{P}(x_{h} = x^{*}) \\ & \stackrel{\text{a.s.}}{=} \mathbb{P}(x_{h} = x^{*}; c^{T}x_{l} = \mathbb{E}_{c \sim \mathcal{C}_{z}}[c^{T}x_{l}|z], \forall x_{l} \in X_{l}) \\ & \stackrel{(4)}{=} \mathbb{P}(x_{h} = x^{*}; \exists x_{h} \in X_{h} : c^{T}x_{h} > 0)\mathbb{P}(\exists x_{h} \in X_{h} : c^{T}x_{h} > 0) \\ & \stackrel{(2,3)}{=} \frac{1}{n_{h}}(1 - (\frac{1}{2})^{n_{h}}), \end{split}$$

where the numbers in brackets refer to the assumptions. When $n_l = n_h = 1$, both probabilities equal $\frac{1}{2}$, while increasing either n_l or n_h decreases $\mathbb{P}(x_l = x^*)$ more than $\mathbb{P}(x_h = x^*)$ which concludes the proof.

We note that Assumption 1 is quite restrictive and could be replaced by something more general:

Assumption 6. Decision set X is finite and a one-to-one mapping $g: X \to Y$ exists such that we get the following alternative formulation of optimization problem (1): $\min_{y \in Y} \mathbb{E}_{c_y \in \mathcal{C}_{y,z}}[c_y|z]$, where $c_y = c^T g^{-1}(y)$.

The proof can be applied in the same way on this alternative formulation. However note that Assumptions 6 and 3 (independence) are contradictory. This means the proof would not hold anymore, but intuitively, biased learning can still occur.

B Application of robust losses to SPO+ and PFYL

In the experiments we train predictive models using SPO+ and PFYL using the proposed robust losses. Since these two approaches are approximations, it is non-trivial to see that these losses can be exactly applied as noted in section 3.4. However due to the structure of the losses, they are readily applied, which we show in detail below.

Let us first introduce the SPO+ gradient Elmachtoub and Grigas [2022]

$$2(x^*(c) - x^*(2\hat{c} - c))$$

and the PFYL gradient Berthet et al. [2020]

$$x^*(c) - \frac{1}{p} \sum_{i=1}^p x^*(\hat{c} + \zeta_i),$$

where ζ_i are drawn from a distribution with a positive and differentiable density (we use $\mathcal{N}(0, \sigma = 1)$ in the experimental results).

Both $l_{\text{top-}k}$ and l_{RO} can be easily adjusted in the mentioned gradients as it only requires substituting $x^*(c)$ by $\frac{1}{k} \sum_{j=1}^{k} x^*_{(j)}(c)$ and $x^*_{\text{RO}}(c)$ respectively. This works similarly for the $l_{k-\text{NN}}$, where it is substituted by $\frac{1}{k} \sum_{j=1}^{k} x^*(c^w_{(j)})$, except that the second term in the SPO+ gradient requires both \hat{c} and c in the evaluation which would result in $\frac{1}{k} \sum_{j=1}^{k} x^*(2\hat{c} - c^w_{(j)})$. To evaluate this exactly the number of evaluations of $x^*(\cdot)$ per data point would be k instead of 1. Because of this we approximate this term with $x^*(2\hat{c} - \frac{1}{k} \sum_{j=1}^{k} c^w_{(j)})$, which in some preliminary experiments showed to be equally effective.

C Further details experimental problems

This section contains further details on the experimental problem classes and the empirical results. First we provide some more details on how the experiments were run in general, followed by more details on the specific problems.

As mentioned in the main article, the experiments were run using *PyEPO* Tang and Khalil [2022]. One main difference is that we included a validation set to pick the best model during training. Based on the results this did not change things significantly, however we believe this is best practice and easy to implement. It positively impacts methods that are prone to over-fitting, so given our claims this positively impacts the approaches trained with empirical losses compared to robust losses.

C.1 Shortest path

Given the pre-specified grid of $(v \times h)$, this problem has v(h-1) + h(v-1) cost values and binary decision variables that make the objective, with constraints allowing only viable paths.

C.2 Travelling salesperson

Euclidean distance is used in between nodes, and since in an optimal decision each arc is only used in one direction, the problem can be modeled as having n(n-1)/2 binary decision variables.

C.3 Energy-cost aware scheduling

Predicting the following day using the previous day the predictive model has 48 features as input and 48 objective coefficients as output. The scheduling problem parameters are equal to the ones used in *Energy-1* by Mandi et al. [2022].

D Table experimental results

Table 1 shows the experimental results as displayed graphically in Section 4.

			2-stage	SPO+				PFYL			
	t	$\overline{\epsilon}$	MSE	emp	RO	top-k	k-NN	emp	RO	top-k	k-NN
SP	100	0.0	16.0 (3.3)	8.9 (1.4)	*8.1 (1.9)	*8.1 (1.4)	*8.0 (1.3)	8.3 (1.0)	*6.4 (1.0)	*7.9 (1.0)	*7.6 (1.0)
	100	0.5	25.2 (3.5)	18.2 (1.8)	*16.8 (1.9)	17.7 (1.7)	*17.1 (1.7)	17.5 (1.6)	*14.8 (1.2)	17.2 (1.5)	*15.7 (1.8)
	100	1.0	67.0 (7.4)	61.3 (3.9)	*58.9 (4.3)	60.3 (4.8)	*56.8 (3.3)	67.3 (4.8)	*61.7 (4.7)	*65.2 (4.4)	*56.1 (4.6)
	1000	0.0	13.0 (2.0)	3.4 (0.8)	×4.3 (0.9)	3.5 (0.9)	×3.8 (0.9)	3.1 (0.6)	×3.5 (0.5)	3.1 (0.6)	3.2 (0.6)
	1000	0.5	19.9 (2.3)	11.0 (1.0)	×11.4 (1.4)	11.1 (1.2)	*10.7 (1.2)	10.1 (0.9)	10.3 (1.1)	10.0 (0.9)	*9.8 (0.9)
	1000	1.0	53.2 (3.3)	46.3 (3.7)	45.7 (2.6)	46.1 (2.8)	*44.3 (3.0)	44.3 (3.1)	43.8 (3.3)	44.1 (3.3)	*41.9 (2.8)
TSP	100	0.0	22.7 (2.2)	9.4 (0.9)	9.4 (1.0)	*8.5 (0.9)	*8.8 (1.1)	8.0 (0.9)	8.1 (0.8)	*5.5 (0.6)	*6.0 (0.6)
	100	0.5	26.5 (2.3)	12.7 (0.9)	12.7 (0.9)	*11.8 (0.9)	12.4 (1.1)	11.8 (1.1)	11.7 (0.9)	*9.2 (0.9)	*9.3 (0.7)
	100	1.0	45.5 (3.3)	32.5 (2.7)	32.6 (2.6)	31.7 (2.8)	30.8 (2.4)	38.9 (3.4)	38.9 (3.3)	*34.4 (2.9)	*29.4 (2.3)
	1000	0.0	21.2 (1.8)	3.9 (0.4)	3.9 (0.4)	3.8 (0.5)	*3.8 (0.4)	2.9 (0.3)	2.9 (0.4)	*2.7 (0.4)	*2.7 (0.3)
	1000	0.5	24.4 (1.8)	7.0 (0.5)	7.0 (0.6)	7.1 (0.5)	*6.9 (0.5)	5.9 (0.4)	5.9 (0.5)	*5.6 (0.4)	*5.6 (0.4)
	1000	1.0	41.4 (2.5)	25.3 (2.0)	25.5 (2.2)	25.3 (2.0)	*23.7 (2.0)	26.8 (2.1)	26.8 (2.0)	*26.3 (2.0)	*22.2 (1.7)
ECAS	100	0.0	6.2 (0.9)	4.0 (1.7)	4.0 (1.6)	3.8 (1.5)	4.0 (1.9)	4.5 (1.5)	4.3 (1.7)	4.3 (1.6)	4.2 (1.8)
	100	0.5	7.7 (1.5)	5.4 (1.5)	5.3 (1.1)	5.5 (1.4)	5.3 (2.0)	5.9 (1.5)	6.4 (1.8)	5.7 (1.9)	5.8 (1.8)
	100	1.0	11.8 (1.7)	8.5 (0.9)	8.9 (2.1)	*8.0 (0.9)	9.3 (1.8)	10.4 (1.9)	9.3 (1.3)	9.8 (2.1)	*8.6 (1.5)
	500	0.0	3.3	2.7	2.8	2.8	2.5	3.5	3.0	4.1	2.9
	500	0.5	4.3	4.1	4.4	4.5	4.1	4.9	6.2	4.7	4.9
	500	1.0	8.3	7.3	9.3	7.0	6.9	8.6	8.8	8.3	7.9

Table 1: Test set mean normalized empirical regret in % (standard deviation). In **bold** the best performing approach and loss combination for each configuration. A * denotes the mean value is significantly better than the same approach trained with the empirical regret loss, a \times denotes when it is significantly worse. Problems are abbreviated: shortest path (SP), traveling salesperson (TSP) and energy-cost aware scheduling (ECAS).