Predict and Optimize: Through the Lens of Learning to Rank

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Abstract

In the last years predict-and-optimize approaches, also known as decision-focused learning, have received increasing attention. In this setting, the predictions of machine learning models are used as estimated cost coefficients in the objective function of a discrete combinatorial optimization problems for decision making. Predict-and-optimize approaches propose to train the ML models, often neural network models, by directly optimizing the quality of decisions made by the optimization solvers. Based on a recent work that proposed a Noise Contrastive Estimation loss over a subset of the solution space, we observe that predict-and-optimize can more generally be seen as a learning-to-rank problem. That is, the goal is to learn an objective function that ranks the feasible points correctly. This approach is independent of the optimization method used and of the form of the objective function. We develop pointwise, pairwise and listwise ranking loss functions, which can be differentiated in closed form given a subset of solutions. We empirically investigate the quality of our generic methods compared to existing predict-and-optimize approaches with competitive results. Furthermore, controlling the subset of solutions allows controlling the runtime considerably, with limited effect on regret.

1 Introduction

Many real-world decision making problems rely on the combination of machine learning (ML) and combinatorial optimization (CO). In those applications, CO problems are solved to arrive at a decision by maximizing or minimizing an objective function. However, often some parameters of the optimization problem, such as costs, prices and profits, are not known but can be estimated from other feature attributes based on historical data.
A two-stage predict-then-optimize approach is widely used by practitioners in both the industry and the public sector, where first an ML model is trained to make point estimates of the uncertain parameters and then the optimization problem is solved using the predictions. However, this treats the parameter errors as independent and does not take the interplay of the parameter errors and their effect on the combinatorial optimisation problem into account. Recently predict-and-optimize \cite{Elmachtoub2021, Wilder2019, Mandi2020} approaches have received increasing attention. In this setting, during training, the ML model is trained with a loss function that first solves the downstream CO problem to observe the joint error. On the technical level, the challenge of integrating combinatorial optimization into the training loop of ML is the non-differentiability of combinatorial problems. To address this, \cite{Mulamba2021} recently proposed an approach motivated by noise-contrastive estimation \cite{Gutmann2010}, where they introduce a new family of surrogate loss functions considering non-optimal feasible solutions as negative examples. In their work, they propose a surrogate loss function, which maximizes the divergence between the objective values of the true optimal and the negative examples.

We argue that predict-and-optimize approach can be more generally viewed through the lens of learning to rank approach \cite{Burges2005}. In a learning to rank (LTR) problem, for each query there is a list of items and their feature variables given. The training objective is to learn a ranking function, which will rank the (top) items correctly for each query.

In the context of CO problems, a partial ordering of the feasible solutions is induced by the objective function. Learning an objective function that orders the feasible solutions hence achieves the goal of predict-and-optimize. When compared to the LTR literature, there are two import differences: 1) part of the structure of the objective function is already given, only some of its parameters must be estimated; and 2) the set of 'items' are all feasible solutions, which are the same for all CO problem instances (queries), but which are intractable to enumerate all. When using backpropagation, 1) needs not be an issue under the assumption that just the objective function itself is differentiable, which is the case for standard continuous functions including linear functions. With respect to 2), we can subsample the feasible solutions as is done in the NCE approach of \cite{Mulamba2021}.

The main contributions of this work are the following: First, we formulate the predict-and-optimize task as a ranking problem. Secondly, we introduce and study several well-known learning to rank loss functions for predict-and-optimize problems. Thirdly, we show that the pairwise ranking loss is a generalization of the loss functions proposed by \cite{Mulamba2021}. Lastly, we show that in case of a linear objective function, the pointwise and pairwise-difference loss functions can be interpreted as trading off the mean square error (MSE) and regret of predictions.

2 Related Literature

**Predict-and-optimize.** Predict-and-optimize forms an interesting class of optimization problems, where the optimization parameters are defined partially. One of the major developments in this topic is the **differentiable optimization layer** \cite{Amos2017}, which analytically computes the gradients by differentiating the KKT optimality conditions of a quadratic program. The gradient calculation of \cite{Amos2017} does not translate to linear programming (LP) problems due to singularities of the objective function in this case. \cite{Wilder2019} address this by introducing a small quadratic regularizer in the objective function while \cite{Mandi2020} introduce a log-barrier regularization term and compute the gradients from the homogeneous self dual embedding of the LP \cite{Ferber2020} studies mixed integer LPs and reduce it to LP by adding cutting plane to the root LP node, applying the framework of \cite{Wilder2019} afterwards. All these methods are specific to the structure of the CO problem used.

Other approaches are independent of the CO problem and solver used. The **smart predict-and-optimize** approach of \cite{Elmachtoub2021} studies optimization problems with linear objectives and where the cost vector has to be predicted. They introduce a convex surrogate upper bound of the loss and propose an easy to use subgradient. \cite{Pogancic2020} also studies problems with linear objectives. They compute the gradient by perturbing the predicted cost vector. For a detailed overview of the predict-and-optimize research development, we refer the readers to \cite{Kotary2021}. 

2
All these approaches involve solving the optimization problem for every loss computation during training, which comes at a very high computational cost. To address this problem, Mulamba et al. [2021] propose contrastive loss functions with respect to a pool of feasible solutions of the optimization problem. It cleanly separates the solving (adding solutions to the pool), from the loss function. This allows the loss function to be differentiated directly. We build on this idea but through the lens of learning to rank.

**Learning to rank.** Learning to rank problems have been studied thoroughly over the years, especially within the context of information retrieval. Readers can refer to Liu [2011] for a detailed analysis. Most of the LTR approaches assign real-valued scores to the items, then define surrogate loss functions on the scores. In pointwise LTR models [Li et al. 2007], the labels are the rank (or true score, if known) of the items. These models fail to consider any inter dependencies across the item rankings. Pairwise ranking approaches [Burges et al. 2005] aim to learn the relative ordering of pairs of items. Finally, listwise approaches [Cao et al. 2007] define loss functions with respect to the scores of the whole ranked lists. The LTR framework has been applied to various contexts such as recommender systems [Karatzoglou et al. 2013] and software debugging [Xuan and Monperrus 2014], among others.

In the predict-and-optimize setting, Demirović et al. [2019] has used LTR, but by considering the parameters of a linear objective function as the items to rank, e.g. the value of items of a knapsack problem, instead of the feasible solutions as we do. Kotary et al. [2021] propose a fair LTR methodology, which impose fairness constraints using constraints in the combinatorial optimization problem and they use predict-and-optimize approaches to integrate the optimization program with an ML model. In contrast, we use LTR models and losses in a predict-and-optimize setting.

### 3 Problem Statement and Motivation

In this section, we introduce the predict-and-optimize setup. We consider a discrete combinatorial optimization problem

\[ v^*(c) \in \arg\min_{v \in V} f(v, c) \]

(1)

where \( V \subseteq \mathbb{Z}^K \) is the set of feasible integer solutions, typically specified implicitly through constraints, and \( f : V \times C \rightarrow \mathbb{R} \) is the real valued objective function, where \( C \subseteq \mathbb{R}^K \) is the domain of the vector of parameters \( c \). We denote an optimal solution of (1) by \( v^*(c) \). The value of \( c \) is unknown but we have access to correlated features \( x \) and a historic dataset \( D = \{(x^i, c^i)\}_{i=1}^N \). The goal is to predict the apriori unknown coefficient vector \( c^i \) in a supervised machine learning setup. To do so, we train a regression model noted by \( m(\omega, x^i) \) to make a prediction of vector \( c^i \), where \( \omega \) are the model parameters. Let us denote the predicted value as \( \hat{c}^i = m(\omega, x^i) \).

In a traditional supervised machine learning setup, we train by minimizing the difference between the elements of vectors \( c \) and \( \hat{c} \). For instance, in a regression problem, we minimize the multi-output mean square error,

\[ \text{mse}(c, \hat{c}) = \sum_{k=1}^K (c_k - \hat{c}_k)^2 = \sum_{k=1}^K \epsilon_k^2 \]

(2)

where \( \epsilon_k = (c_k - \hat{c}_k) \), over a set of \( N \) instances \( \{(c, \hat{c})\} \).

In contrast, in the predict-and-optimize setup \( \hat{c} \) is an intermediate result. The final output is \( v^*(\hat{c}) \), the solution of the discrete combinatorial optimization problem. The final goal is to minimize the impact of the solution \( v^*(\hat{c}) \) in the downstream optimization problem whenever the real cost vector \( c \) is realized. In order to measure how good \( \hat{c} \) is, we compute the regret of the combinatorial optimisation. The **regret** is defined as the difference between the value of the optimal objective value \( f(v^*(c), c) \) and the value of the objective function with ground truth \( c \) and predicted solution \( v^*(\hat{c}) \). Formally, we define regret, without any assumptions on the structure of \( f \), as

\[ \text{Regret}(\hat{c}, c) = f(v^*(\hat{c}), c) - f(v^*(c), c) \]

(3)

Ideally, we aim to learn parameters \( \omega \) that determine \( \hat{c} = m(\omega, x) \) such that it minimizes the regret. To do so in a neural network setup, the gradient of the regret has to be backpropagated, which requires
computing the exact derivative of the Regret (5). This task is problematic as \( V \) is discrete and the Regret function is non-continuous and involves differentiating over the argmin in \( v^*(\hat{c}) \).

To accomplish this challenge, a typical approach for predict-and-optimize is to formulate a differentiable and efficient-to-compute surrogate loss function \( \mathcal{L}(\cdot) \) that considers the structure of the underlying optimisation problem.

As mentioned in section 2, several recent works have studied this problem. However, in all those cases, in order to compute the gradient, the optimization problem (1) must be solved repeatedly for each instance during training. Hence, scalability is a major challenge in these approaches.

### 3.1 Contrastive Surrogate Loss

To improve the scalability of predict-and-optimize \cite{Mulamba2021} proposed an alternative class of loss functions, which can be differentiated in closed-form without solving the combinatorial problem. Motivated by noise contrastive estimation \cite{Mikolov2013}, they propose an NCE loss by considering a set of (possibly) non-optimal feasible solutions as negative samples. This set of feasible solutions is denoted by \( S \subset V \). Then, by proposing the exponential distribution \( p(v; c) = \frac{1}{Z} \exp \left( -f(v, c) \right) \) they derive the following NCE loss \cite{Mulamba2021}:

\[
\mathcal{L}_{NCE}(\hat{c}, c) = \frac{1}{|S|} \sum_{v \in S} \left( f(v^*(c), \hat{c}) - f(v^*, \hat{c}) \right). \tag{4}
\]

The novelty of this approach is that Eq. (4) is differentiable and that the differentiation does not involve solving the optimization problem in (1). Further, if the solutions in \( S \) are optimal solutions of arbitrary cost vectors, this approach is equivalent to training in a region of the convex-hull of \( V \).

### 4 Rank Based Loss Functions

In this section we develop and motivate a family of surrogate loss functions for predict-and-optimize problems. We remark that, for a given \( c \), we can create a partial ordering of all \( v \in V \) by ordering them with respect to the objective value. Let us denote by \( p_1, \ldots, p_{|V|} \) the indices of \( V \) so that \( f(v^{p_1}, c) \leq f(v^{p_2}, c) \leq \ldots \leq f(v^{p_{|V|}}, c) \). The idea of our approach is to generate prediction \( \hat{c} \) so that \( f(v^{p_1}, \hat{c}) \leq f(v^{p_2}, \hat{c}) \leq \ldots \leq f(v^{p_{|V|}}, \hat{c}) \). Notice that, if the ranks of \( v \in V \) with respect to \( \hat{c} \) are identical to that of \( c \), the regret is zero. Furthermore, it is sufficient that \( \forall p_s : f(v^{p_1}, \hat{c}) \leq f(v^{p_s}, \hat{c}) \) for the regret to be zero. In general, our surrogate task is to learn the ranking of each \( v \in V \) with respect to \( c \). This motivates us to use the LTR framework to develop a new class of surrogate loss functions for predict-and-optimize problems.

Drawing a parallel to the LTR literature, we consider each \( x \) a query, and the feasible solutions \( v \in V \) as the set of items to be ordered. Our formulation differs from traditional LTR framework because in LTR problems each item has its own set of feature variables, whereas in our formulation each \( v \) does not have feature variables. We hence only have query-features (\( x \) itself) to predict \( c \). In the LTR framework, a ranking function is used to assign scores to each item. In predict-and-optimize setup, the objective function \( f(v, c) \) determines the score, and our goal is to learn the cost vector \( c \) leading to a scoring function with a good ranking.

To rank all \( v \in V \) is an intractable task for most combinatorial problems. To overcome this in practice, we will consider a set of feasible solution \( S \subset V \). The proposed implementation is described in pseudocode form in Algorithm 1. For each \( c \), we compute a loss function \( L_c(\hat{c}, c) \) considering the surrogate ranking task. The implementation details are described later.

#### 4.1 Pointwise Ranking

In a pointwise ranking loss, the loss function is defined for each item (feasible solution) independently. In our pointwise rank loss formulation, we propose to regress the predicted objective function value on the actual objective function value. Thus, we propose the pointwise loss function

\[
L_P(\hat{c}, c; S) = \frac{1}{|S|} \sum_{v \in S} (f(v, \hat{c}) - f(v, c))^2 \tag{5}
\]

that measures the errors in the evaluation of the predicted cost function at each point in \( S \).
Algorithm 1 Gradient-descent implementation of predict-and-optimize problems with Ranking Loss

Input: \( D = \{(x_i, c_i)\}_{i=1}^{n} \)

1: Initialize \( \omega \)

2: Initialize \( S = \{v^*(c_i) \mid (x_i, c_i) \in D \} \)

Training

3: for each epochs do
4:     for each \((x_i, c_i)\) do
5:         \( \hat{c}_i = m(\omega, x_i) \)
6:         if random() \(< p_{\text{solve}} \) then
7:             \( v^*(\hat{c}_i) \leftarrow \text{call solver to solve Eq. (1)} \)
8:             \( S \leftarrow S \cup \{v^*(\hat{c}_i)\} \)
9:         end if
10:     end for
11: end for
12: \( \omega \leftarrow \omega - \alpha \frac{\partial L}{\partial \omega} \) # backward pass
13: end for

Intuitive idea of the pointwise loss function. When the objective function is linear i.e. \( f(v, c) = c^T v \), the pointwise loss (5) becomes

\[
L^p(\hat{c}, c; S) = \frac{1}{|S|} \sum_{v \in S} (c^T v - \hat{c}^T v)^2
\]

The derivative of this loss is

\[
\frac{\partial L^p(\hat{c}, c; S)}{\partial \hat{c}} = -\frac{2}{|S|} \sum_{v \in S} (c^T v - \hat{c}^T v) v
\]

When considering a combinatorial problem where \( v \) is a binary vector, we can see from Eq. (7) that coordinates where \( v \) has zeros, will not contribute to the gradient. Moreover, the first component \( (c^T v - \hat{c}^T v) \) is the difference between the actual and the predicted objective value on \( v \). The gradient contribution of \( v \) is weighed by this difference.

Pointwise loss as a regularizer. For the special case of a linear objective function \( f(v, c) = \sum_{j=1}^{K} c_j v_j \), the pointwise task loss can be rewritten as:

\[
L^p(\hat{c}, c; S) = \sum_{i=1}^{K} (\hat{c}_i - c_i)^2 + \sum_{i \neq j} (\hat{c}_i - c_i)(\hat{c}_j - c_j) \gamma_{ij}
\]

\[
= \sum_{i=1}^{K} \epsilon_i^2 \gamma_i + \sum_{i \neq j} \epsilon_i \epsilon_j \gamma_{ij}
\]

where \( \gamma_i = \frac{1}{|S|} \sum_{v \in S} v_i^2 \) and \( \gamma_{ij} = \frac{1}{|S|} \sum_{v \in S} v_i v_j \) and \( \epsilon_i \) defined as in (2). In this case, it is a weighted version of the \( \text{mse} \) function plus a term that measures the pairwise relationship of errors of the coordinates.

Moreover, when \( V \subseteq \{0, 1\}^K \), the weight \( \gamma_i \) is the frequency of how many times coordinate \( v_i \) takes value 1 (since \( v_i^2 = v_i \)). Coefficients \( \gamma_{ij} \) measure the frequency where \( v_i \) and \( v_j \) take value 1 at the same time. In particular, if \( S = V \)

\[
L^p(\hat{c}, c; V) = \frac{1}{2} \left( \text{mse}(\hat{c}, c) + \sum_{i=1}^{K} \sum_{j=1; j < i}^{K} \epsilon_i \epsilon_j \right)
\]

Hence, the pointwise loss function can be seen as the \( \text{mse} \) plus a regularizer which penalizes the crossed-errors between coordinates of the vector \( c \).
4.2 Pairwise Ranking

Let \((p, q)\) be an ordered pair in \(S\) with respect to \(c\). We define \(OP^S_{c}\) as the set of all the ordered pairs such that the first coordinate dominates the second one in the order induced by \(c\), or equivalently:

\[(p, q) \in OP^S_{c} \iff f(v^p, c) < f(v^q, c)\]  

(9)

For an ordered pair \((p, q)\), we expect the predicted \(\hat{c}\) would also respect the ordering i.e. \(f(v^p, \hat{c}) < f(v^q, \hat{c})\). In other words, \(f(v^p, \hat{c}) - f(v^q, \hat{c})\) is the quantity we aim to minimize. This gives us the following loss

\[
\frac{1}{|\text{OP}^S_{c}|} \sum_{(p,q) \in \text{OP}^S_{c}} (f(v^p, \hat{c}) - f(v^q, \hat{c}))
\]

(10)

We point out that (10) takes the form of (4), when \(\text{OP}^S_{c} = \{(v^*(c), v^*) | s \in S\}\). This shows that the NCE approach of [Mulamba et al., 2021], although derived differently, can be seen as a special case of a best-versus-rest pairwise approach.

In the standard pairwise margin ranking loss formulation [Joachims, 2002], we do not penalize if \(f(v^p, \hat{c})\) is smaller than \(f(v^q, \hat{c})\) by at least a margin of \(\nu > 0\). In this paper, we hence use the following generic pairwise loss

\[
\frac{1}{|\text{OP}^S_{c}|} \sum_{(p,q) \in \text{OP}^S_{c}} \max (0, \nu + f(v^p, \hat{c}) - f(v^q, \hat{c}))
\]

(11)

Ordered pairs generation. Eq. (11) is built upon the concept of a pairwise ranking loss [Burges et al., 2005]. Note that, to implement this approach we have to identify ordered pairs from the negative examples. Clearly generating all possible pairs comes with a complexity of \(O(|S|^2)\).

We hence consider the same best-versus-rest scheme as we derived from the NCE loss, i.e. \(\text{OP}^S_{c} = \{(v^{p_1}, v^{p_2}), (v^{p_3}, v^{p_4}), \ldots, (v^{p_{|S|-1}}, v^{p_{|S|}})\}\). Other schemes are possible too.

Example. To demonstrate the shortcoming of the pointwise loss and the motivation behind the pairwise loss formulation, we construct a simple example. Let us consider the feasible space is the 2 dimensional 0-1 space, containing the four feasible points \([0, 0], [0, 1], [1, 0], [1, 1]\). Now, let \(c\) be \([2, -3]\). The objective values at these four points are 0, -5, 2 and -3, hence \(v^*(c) = [0, 1]\). Now let \(\hat{c}_1 = [-1, 1]\) and \(\hat{c}_2 = [5, -11]\). For \(\hat{c}_1\) and \(\hat{c}_2\), the objective values of these four points are 0, 1, -1, 0 and 0, -11, 5, -6 respectively. The square error of both \(\hat{c}_1\) and \(\hat{c}_2\) is 45 = \(3^2 + 6^2\). The pointwise loss between \(c\) and \(\hat{c}_1\) is 54 = \((0 + (-5 - 1)^2) + (2 + 1)^2 + (-3 - 0)^2\) and \(c\) and \(\hat{c}_2\) is 54 = \((0 + (-5 + 11)^2) + (2 - 5)^2 + (-3 + 6)^2\). But \(v^*(\hat{c}_1) = [1, 0]\) and \(v^*(\hat{c}_2) = [0, 1]\) = \(v^*(c)\). Even though the regret of \(\hat{c}_2\) is 0, its pointwise loss is the same as \(\hat{c}_1\), whose regret is positive.

For computing the pairwise loss, first, we have to generate the ordered pairs. The ordering of the feasible points with respect to \(c\) is \([0, 1], [1, 1], [0, 0], [1, 0]\). Following the best-vs-rest scheme, the pairs are \(\{(0, 1), (1, 1), (0, 0), (1, 0)\}\). For \(\hat{c}_1\) the value of the pairwise loss is \(1 + 1 + 2 = 4\). For \(\hat{c}_2\) the value of pairwise loss is \(0 + 0 + 0 = 0\), which is reasonable as its regret is 0.

4.3 Regress on Pairwise Difference

Another way to generate a ranking of solutions in \(S\) is to generate predicted cost vectors, that produce the same \textit{difference} in objective value. To do so, we propose a loss function over the difference over pairs of solutions their cost vectors \(c_i\) and \(\hat{c}_i\). This loss function can be formulated as:

\[
L_{pd}(\hat{c}, c; S) = \frac{1}{|S|} \sum_{(p,q) \in \text{OP}^S_{c}} \left( (f(v^p, \hat{c}) - f(v^q, \hat{c})) - (f(v^p, c) - f(v^q, c)) \right)^2
\]

(12)
For the sake of clarity, we omitted O.P.\textsuperscript{S} from the definition of $L_p d$.

It is easy to check that in the case of a linear objective:

$$L_p d(\hat{c}, c; S) = \sum_{i=1}^K \epsilon_i \gamma_i + \sum_{i \neq j} \epsilon_i \epsilon_j \gamma_{ij}$$

where $\gamma_i = \frac{1}{|S|} \sum_{(p,q) \in S} (v_i^p - v_i^q)^2$, which is proportional to how many times $v_i^p$ and $v_i^q$ are different, and $\gamma_{ij} = \frac{1}{|S|^2} \sum_{(p,q) \in S} (v_i^p - v_j^q)(v_i^q - v_j^p)$. As in the pointwise loss, the pairwise difference loss can be seen as a weighted \textit{mse} loss function with a regularizer term; this time involving the difference between solutions rather than individual coefficients.

**Example continued.** As before, the set of pairs is $\{(0,1), (1,1), (0,0), (0,1), (1,0)\}$. The difference between these three sets of pairs for $c$ are 2, 5, 7. The corresponding differences for $\hat{c}_1$ and $\hat{c}_2$ are $-1, -1, -2$ and $5, 11, 16$. So, the corresponding losses for $\hat{c}_1$ and $\hat{c}_2$ are $(2 + 1)^2 + (7 + 2)^2 = 94$ and $(2 - 5)^2 + (5 - 11)^2 + (7 - 16)^2 = 94$.

| Pointwise | Pairwise | Pairwise-diff | Listwise | NCE | MAP | SPO | Blackbox | Two-stage |
|-----------|----------|---------------|----------|-----|-----|-----|----------|-----------|
| Deg-1     | 14.01%   | 12.67%        | 13.42%   | 13.29% | 26.35% | 13.09% | 12.90%   | 13.36%    | 12.55%    |
| Deg-2     | 23.27%   | 22.77%        | 22.55%   | 21.62% | 54.88% | 21.36% | 21.96%   | 22.63%    | 23.13%    |
| Deg-4     | 71.78%   | 70.92%        | 78.31%   | 68.91% | 218.64% | 88.46% | 71.21%   | 72.97%    | 72.98%    |
| Deg-8     | 503.70%  | 364.08%       | 409.42%  | 414.75% | 2300%  | 1115%  | 461.04%  | 768.54%   | 416.91%   |

The difference between solutions rather than individual coefficients.

| Energy-1  | 3.61%    | 1.31%        | 1.38%    | 1.43%  | 18.76% | 1.48%  | 1.40%    | 1.50%     | 1.57%     |
| Energy-2  | 2.93%    | 1.80%        | 1.80%    | 1.81%  | 31.92% | 1.79%  | 1.90%    | 1.79%     | 2.00%     |

| Matching-1| 91.30%   | 89.67%       | 89.50%   | 89.57% | 88.39% | 89.07% | 88.84%   | 89.63%    | 94.24%    |
| Matching-2| 90.51%   | 88.22%       | 90.50%   | 87.68% | 87.18% | 85.05% | 89.46%   | 89.33%    | 94.11%    |

Table 1: Comparison of regret on three problem sets. We present average percentage regret of 10 runs.

### 4.4 Listwise Ranking

Instead of considering instance pairs, the Listnet loss [Cao et al., 2007] considers the entire ordered list. It is obvious that, if the list contains only two instances, then there are no differences between the two approaches. The Listnet loss computes the probabilities of each item being the top one and then defines a cross entropy loss of these probabilities. In our context, we first define the probability distribution of $v \in V$ being the top one. The most natural distribution is the exponential distribution also used for the NCE loss [Mulamba et al., 2021]:

$$p(v|c) = \frac{\exp(-f(v,c))}{\sum_{v' \in V} \exp(-f(v',c))} \quad (14)$$

It is easy to verify that, if $v$ is one minimizer of Eq. [1] then it will maximize Eq. [14]. Instead of using NCE to avoid the computation of the partition function (denominator), we will approximate it as in the ranking functions proposed above, namely to replace $V$ by a subset $S \subseteq V$.

Given a probability distribution, Listnet uses the cross entropy loss between $p(v|c)$ and $p(v|\hat{c})$ for all $v \in S$:

$$L_S'(\hat{c}, c) = -\frac{1}{|S|} \sum_{v \in S} p(v|c) \log p(v|\hat{c}) \quad (15)$$

### 4.5 Implementation

So far we define pointwise [5], pairwise [11], pairwise-difference [12] and listwise [15] ranking losses. With these proposed ranking loss definitions, we will implement end-to-end training of
predict-and-optimize problems. As mentioned, the fundamentals of the LTR loss functions is to learn the partial ordering of \( v \in S \). To create this set of feasible solutions \( S \), we first initialise it with all true optimal solutions, as done by Mulamba et al. [2021]. Following their methodology, we could also choose to dynamically expand \( S \). To do so we define a hyperparameter \( p_{\text{solve}} \), which is the probability of calling a optimization oracle to solve an instance during training. If an instance is solved, its solution is added to \( S \). Obviously with \( p_{\text{solve}} = 100\% \), we solve Eq. (1) for every \( \hat{c}_i \) during training. This is the baseline approach, and we investigate the effect of a lower \( p_{\text{solve}} \) in the experiments.

The generic structure of the proposed algorithm is shown in Algorithm 1, which is a modified version of standard gradient descent algorithms for predict-and-optimize problems. Instead of a standard ML loss (like squared error or cross entropy), we use the proposed ranking losses for training the network. To implement the ranking loss, \( S \) is initialized by caching all the optimal solutions of the training instances in line 2 and in line 8. \( S \) is expanded with probability \( p_{\text{solve}} \). The distinctive feature of this proposed approach is that the loss function \( L(\hat{c}_i, c_i) \) does not involve any argmin differentiation. So we can use standard automatic differentiation libraries and it can be run on GPU. Yet, it still considers the task loss of the downstream optimization problem.

### 5 Experiments

We analyze our approaches on a series of experiments. We consider three discrete combinatorial optimization problems. First, we briefly describe the experimental setups.

#### Shortest Path Problems.

We adopt this synthetic experiment from Elmachtoub and Grigas [2021]. It is a shortest path problem in a 5 \( \times \) 5 grid, with the objective of going from the southwest corner of the grid to the northeast corner where the edges can go either north or east. The feature vectors are...
sampled from a multivariate Gaussian distribution. We follow their model to generate the cost vector

\[ c_{ij} = \left( \frac{1}{\sqrt{p}} (Bx_i) + 1 \right)^{\text{Deg}} \epsilon_i^j \]  

(16)

where \( c_{ij} \) is the \( j \)-th component of cost vector \( c_i \) and \( B \) is the latent data generation matrix. \( \text{Deg} \) specifies the extent of model specification, the higher the value of \( \text{Deg} \), the more it deviates from a linear model and the more errors there will be. We experiment with degree of 1, 2, 4 and 8. For each degree, we generate 1000 instances; out of which 800, 50 and 150 are used for training, validation and test purposes. The underlying model is a neural network without any hidden layer i.e. a regression model.

**Energy-cost Aware Scheduling.** Next we consider the problem of energy-cost aware scheduling, adapted from CSPLib [Gent and Walsh 1999], a library of constraint optimization problems. In energy-cost aware scheduling [Simonis et al. 1999], a given number of tasks, each having its own duration, power usage, resource requirement, earliest possible start and latest-possible end, must be scheduled on a certain number of machines without violating the resource capacities of each machine. A task cannot be stopped or migrated once started on a machine. The goal of the optimization problem is to find the scheduling which would minimize the total energy consumption. But energy prices are not known, as they would happen in the future. The prediction task is to predict the future energy prices using feature variables such as calendar attributes; day-ahead estimates of weather characteristics; SEMO day-ahead forecasted energy-load, wind-energy production and prices. We took the energy price data from [Ifrim et al. 2012], which contains historical energy price data at 30-minute intervals from 2011-2013. We study two instances named Energy-1 and Energy-2. The first one involves scheduling 3 tasks on 10 machines, whereas the other instance has 3 tasks and 15 machines.

![Figure 2: Change of MSE and Regret with \( \alpha \) as a tuning parameter. The green and blue bar present the MSE loss and percentage regret respectively.](image)

**Diverse Bipartite Matching.** We adopt this from [Ferber et al. 2020] and [Mulamba et al. 2021]. The topologies are taken from the CORA citation network [Sen et al. 2008]. We have 27 disjoint topologies and each of them is considered as an instance. The prediction task is to predict which edges are present. Each node has 1433 bag-of-words features. The feature of and edge is formed by concatenating features of the two corresponding nodes. The optimization task is to find the maximum matching after prediction. In the optimization task, diversity constraints ensures that there are some edges between papers of the same field as well as edges between papers of different fields. We study two instantiations with different degrees of diversity constraints (see Appendix for detail).

### 5.1 Experimental Results

**Performance of surrogate loss functions.** In this section, we compare the quality of ranking based surrogate loss functions. We compare the ranking based loss functions with the SPO model [Elmachtoub and Grigas 2021], Blackbox model [Pogancic et al. 2020] and the NCE and MAP approach.
of Mulamba et al. [2021]. We also include a two-stage baseline approach which is trained purely on MSE loss. Table 1 lists the detailed result for the shortest path problem, energy scheduling and diverse bipartite matching problem. In Table 1, we report the percentage regret \( \left( \frac{f(v^*(c), c) - f(v^*(c), c)}{f(v^*(c), c)} \right) \) of the above mentioned approaches for the three problems.

For the shortest path problem, we see the regret goes up with the degree parameter. This is expected as the degree parameter controls the magnitude of the errors of the linear model. For degree 1, the two-stage model performs best as the linear model represents the data generation process perfectly. For degree 2 and 4, the listwise loss function does the best among the proposed loss functions and is comparable to other predict-and-optimize models. For the scheduling problem, the pairwise loss is the best one for Energy-1 and only 0.01% behind the best one for Energy-2. For the matching problem, the regret is higher as the ML problem itself is challenging. In both cases the NCE model does best, even though it had poorer performance on the other problems. The pairwise and the listwise approach are comparable; they both do do better than SPO and Blackbox for Matching-2. In all cases the pointwise loss function performs poorly, even worse than pure MSE (two-stage). The possible explanation is that its added penalty term is not always aligned with regret as discussed in section 4.2.

| p_solve | Pointwise | Pairwise | Pairwise-diff | Listwise |
|---------|-----------|----------|---------------|----------|
|         | Regret | Time (s) | Regret | Time (s) | Regret | Time (s) | Regret | Time (s) |
| Energy-1 | 100%  | 3.61% | 55 | 1.32% | 50 | 1.38% | 55 | 1.43% | 47 |
| 10% | 3.20% | 18 | 1.29% | 20 | 1.37% | 20 | 1.47% | 18 |
| Energy-2 | 100%  | 2.93% | 80 | 1.80% | 72 | 1.80% | 77 | 1.81% | 65 |
| 10% | 3.24% | 35 | 1.84% | 22 | 1.81% | 25 | 1.82% | 22 |

Table 2: Impact of p_solve on per epoch training time and regret in Energy scheduling instances

**MSE vs Regret tradeoff.** The motivation behind predict-and-optimize approach is that by minimizing MSE it is not always possible to minimize regret. The three problems we consider happen all to be integer linear programming (ILP) problems. As ILP problems are scale-invariant, the regret can be minimized even if the predictions are multiples of the actual values. As the pairwise (and listwise) loss only consider the ordering, they can achieve arbitrarily bad MSE. On the other hand, the pointwise approach and the pairwise-difference approach take the actual difference into consideration, so, we can expect these two approaches to have lower MSE.

In Figure 2, we show both MSE and regret of the predictions. In all cases we observe that the MSE loss of the pointwise loss is lower than the other LTR bases loss functions. But its regret is even higher than MSE, as seen before. The pairwise difference loss function has marginally better MSE than listwise and pairwise losses, showing little added gain from its more MSE-related formulation.

**Combined Regression and Ranking Experiment.** The previous experiment reveals that although the performances of the ranking loss functions are comparable with the state-of-the-arts in terms of regret, their MSE loss remains high. In this experiment we will consider a convex combination of MSE loss and pairwise ranking loss, inspired by Sculley [2010] but formulated as a multi-task problem instead of sampling between the two losses:

\[
\alpha L_{\text{OP}}(\hat{c}, c) + (1 - \alpha) \text{mse}(\hat{c}, c)
\]

(17)

The motivation behind this loss function is that we can control \( \alpha \) as a tuning parameter. Clearly, \( \alpha = 0 \) results in MSE loss whereas \( \alpha = 1 \) results in pairwise ranking loss.

Figure 2 displays the impact \( \alpha \) on the two scheduling instances. As hypothesised, we see MSE goes up and regret goes down as we increase \( \alpha \). This experiment suggests it is possible to choose a value of \( \alpha \) so that we sacrifice regret (problem-specific) to attain predictions with lower MSE (close to the true values).

**Impact of \( p_{\text{solve}} \).** In our next experiment, we change the value of \( p_{\text{solve}} \). This would make the training faster because of two reasons. Firstly, we have to call the optimization oracle few number of times. Secondly, the smaller cardinality means ranking loss would be computed on fewer datapoints. In Table 2 we report percentage regret and per epoch runtime of the four ranking loss functions for \( p_{\text{solve}} = 10\% \) and \( 100\% \) for the scheduling instances. We choose this problem because this is most
difficult optimization problem among the three. Table 2 shows that in all cases, reducing $p_{\text{solve}}$ to 10% barely impacts regret for all except pointwise (which already performs worse). On the other hand, the efficiency gain in terms of runtime is significant.

6 Conclusion

We framed the predict-and-optimize problem as a learning to rank problem. This generalizes the approach of [Mulamba et al., 2021] and inherits its nice properties of separating the solving from the loss computation. It also allows to draw connections between the two-stage MSE loss and regret minimizing ranking losses. This stimulates a further cross fertilisation of the rich and more mature field of learning to rank with the relatively recent topic of predict-and-optimize.

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A Problem Specification

A.1 Shortest Path Problem

In this problem, we consider shortest path problem on $5 \times 5$ a grid. The goal is to go from the southwest corner to the northeast corner, where we can go towards east or north. We model it as an LP problem.

$$\min_{x \geq 0} c^\top x$$

subject to

$$Ax = b$$

Where $A$ is the incidence matrix. The decision variable $x$ is binary vector whose entries would be 1 only if corresponding edge is selected for traversal. $b$ is 25 dimensional vector whose first entry is 1 and last entry is -1 and rest are 0. The constraint must be satisfied to go from the southwest corner to the northeast corner. With respect to the (predicted) cost vector $c \in \mathbb{R}^{|E|}$, the objective is to minimize the cost.

A.2 Energy-cost Aware Scheduling

In this problem, $J$ is the set of tasks to be scheduled on $M$ number of machines maintaining resource requirement of $R$ resources. The tasks must be scheduled over $T = 48$ set of equal length time periods. Each task $j$ is specified by its duration $d_j$, earliest start time $c_j$, latest end time $l_j$, power usage $p_j,u_{jr}$ is the resource usage of task $j$ for resource $r$ and $c_{mr}$ is the capacity of machine $m$ for resource $r$. Let $x_{jmt}$ be a binary variable which is 1 only if task $j$ starts at time $t$ on machine $m$. If $c_t$ is the (predicted) energy price at timeslot $t$, the objective is to minimize the following formulation of total energy cost. Then the problem can be formulated as the following MILP:

$$\min_{x_{jmt}} \sum_{j \in J} \sum_{m \in M} \sum_{t \in T} x_{jmt} \left( \sum_{t' \leq t + d_j} p_j c_{t'} \right)$$

subject to

$$\sum_{m \in M} \sum_{t \in T} x_{jmt} = 1, \forall j \in J$$

$$x_{jmt} = 0 \ \forall j \in J \forall m \in M \forall t < c_j$$

$$x_{jmt} = 0 \ \forall j \in J \forall m \in M \forall t + d_j > l_j$$

$$\sum_{j \in J} \sum_{t \leq t'} x_{jmt} u_{jr} \leq c_{mr}, \forall m \in M \forall r \forall t \in T$$

The first constraint ensures each task is scheduled only once. The next constraints ensure the task scheduling abides by earliest start time and latest end time constraints. The final constraint is to respect the resource requirement of the machines.

A.3 Diverse Bipartite Matching

We adapt this from [Ferber et al., 2020]. In this problem 100 nodes representing scientific publications are split into two sets of 50 nodes $N_1$ and $N_2$. A (predicted) reward matrix $c$ indicates the likelihood that a link between each pair of nodes from $N_1$ to $N_2$ exists. Finally a indicator $m_{i,j}$ share the same subject field, and 0 otherwise $\forall i \in N_1, j \in N_2$. Let $p \in [0, 1]$ be the rate of pair sharing their field in a solution and $q \in [0, 1]$ the rate of unrelated pairs, the goal is to match as much nodes in $N_1$ with at most one node in $N_2$ by selecting edges which maximizes the sum of rewards under similarity and diversity constraints. Formally:

$$\max_x \sum_{i,j} c_{i,j} x_{i,j}$$

subject to

$$\sum_{i,j} x_{i,j} \leq 1 \ \forall i \in N_1$$

$$\sum_{i,j} x_{i,j} \leq 1 \ \forall j \in N_2$$

$$\sum_{i,j} m_{i,j} x_{i,j} \geq p \sum_{i,j} x_{i,j} \ \forall i \in N_1, j \in N_2$$

$$\sum_{i,j} (1 - m_{i,j}) x_{i,j} \geq q \sum_{i,j} x_{i,j} \ \forall i \in N_1, j \in N_2$$

$$x_{i,j} \in \{0, 1\} \ \forall i \in N_1, j \in N_2$$

In our experiments, we considered two variations of this problem with $p = q = 0.25$ and 0.05, respectively named Matching-1 and Matching-2.