
Decision-Focused Learning: Through the Lens of Learning to Rank

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Abstract

In the last years, decision-focused learning, also known as predict-and-optimize, has received increasing attention. In this setting, the predictions of a machine learning model are used as estimated cost coefficients in the objective function of a discrete combinatorial optimization problem for decision making. Decision-focused learning proposes 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 decision-focused learning can more generally be seen as a learning-to-rank problem, where the goal is to learn an objective function that ranks the feasible points correctly. This observation 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 decision-focused learning 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 *decision-focused learning* (Wilder et al., 2019; Pogancic et al., 2020) (also known as predict-and-optimize (Elmachoub & Grigas, 2021; Mandi et al., 2020)) has 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, Mulamba et al. (2021) recently proposed an approach motivated by noise-contrastive estimation (Gutmann & Hyvärinen, 2010), 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 decision-focused learning can be more generally viewed through the lens of learning to rank (LTR) approach (Borges et al., 2005). In a 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 the orders of the feasible solution with respect to the objective function hence achieves the goal of decision-focused learning. When compared to the LTR literature, there are two important 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

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solutions, which are the same for all CO problem instances (queries), but it is intractable to enumerate all. While back-propagating, 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 by [Mulamba et al. \(2021\)](#).

The main contributions of this work are the following: First, we formulate the decision-focused learning as a ranking problem. Secondly, we introduce and study several well-known learning to rank loss functions. In particular, we formulate pointwise, pairwise and listwise ranking loss functions for decision-focused learning problems. Thirdly, we show that the pairwise ranking loss is a generalization of the loss functions proposed by [Mulamba et al. \(2021\)](#). 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

Decision-focused learning. Decision-focused learning involves optimization problems, where the optimization parameters are defined partially. One of the major developments in this topic is the *differentiable optimization layer* ([Amos & Kolter, 2017](#)), which analytically computes the gradients by differentiating the KKT optimality conditions of a quadratic program. The gradient calculation of [Amos & Kolter \(2017\)](#) does not translate to linear programming (LP) problems due to singularities of the objective function in this case. [Wilder et al. \(2019\)](#) address this by introducing a small quadratic regularizer in the objective function while [Mandi & Guns \(2020\)](#) introduce a log-barrier regularization term and compute the gradients from the homogeneous self dual embedding of the LP. [Ferber et al. \(2020\)](#) studies mixed integer LPs and reduce it to LP by adding cutting plane to the root LP node, applying the framework of [Wilder et al. \(2019\)](#) 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 [Elmachtoub & Grigas \(2021\)](#) 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. [Pogancic et al. \(2020\)](#) also studies problems with linear objectives. They compute the gradient by perturbing the predicted cost vector. [Niepert et al. \(2021\)](#) extend this work by adding noise-perturbations for perturbation-based implicit differentiation. For an overview of decision-focused learning, we refer the readers to [Kotary et al. \(2021\)](#).

All these approaches involve solving the optimization problem for every instance 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 & Monperrus, 2014](#)), among others.

[Demirović et al. \(2019\)](#) have used LTR in decision-focused learning framework, 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 decision-focused learning to integrate the optimization program with an ML model. In contrast, we use LTR models and losses for decision-focused learning.

3. Problem Statement and Motivation

In this section, we introduce the decision-focused learning setup. We consider a discrete combinatorial optimization problem

$$v^*(c) \in \underset{v \in V}{\operatorname{argmin}} f(v, c) \quad (1)$$

where $V \subseteq \mathbb{Z}^K$ is the set of *feasible* integer solutions, typically specified implicitly through constraints, and $f : V \times \mathcal{C} \rightarrow \mathbb{R}$ is the real valued objective function, where $\mathcal{C} \subset \mathbb{R}^K$ 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 model noted by $m(\omega, x_i)$ to make a prediction of vector c_i , where ω 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 c and \hat{c} . For instance, in a regression problem, we minimize the multi-output mean square error,

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

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

In contrast, in decision-focused learning \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

$$\text{Regret}(\hat{c}, c) = f(v^*(\hat{c}), c) - f(v^*(c), c). \quad (3)$$

Ideally, we aim to learn parameters ω 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 (3). This task is problematic as V is discrete and the regret function is non-continuous and involves differentiating over the argmin in $v^*(\hat{c})$.

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 decision-focused learning [Muller et al. \(2021\)](#) proposed an alternative class of loss functions. They first define the following probability distribution of $v \in V$ being the optimal one.

$$p(v|c) = \begin{cases} \frac{\exp(-f(v, c))}{\sum_{v' \in V} \exp(-f(v', c))} & \text{if } v \in V \\ 0, & \text{if } v \notin V \end{cases} \quad (4)$$

It is easy to verify that, if v is one minimizer of Eq. 1, then it will maximize Eq. 4. To define the loss functions they consider to have access to S , a *subset* of V and treat

$(S \setminus \{v^*(c)\})$ as negative examples. With this setup, they define the following noise contrastive estimation (NCE) loss

$$L_{\text{NCE}}(\hat{c}, c) = \frac{1}{|S|} \sum_{v^s \in S} (f(v^*(c), \hat{c}) - f(v^s, \hat{c})). \quad (5)$$

The novelty of this approach is that Eq. (5) 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 decision-focused learning 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 $p_1, \dots, p_{|V|}$ the indices of V so that $f(v^{p_1}, c) \leq f(v^{p_2}, c) \leq \dots \leq f(v^{p_{|V|}}, c)$. The key idea of our approach is to generate prediction \hat{c} so that $f(v^{p_1}, \hat{c}) \leq f(v^{p_2}, \hat{c}) \leq \dots \leq f(v^{p_{|V|}}, \hat{c})$. 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 decision-focused learning 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 decision-focused learning setup, we will consider the objective function $f(v, c)$ as the scoring function.

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 $L(\hat{c}, c)$ considering the surrogate ranking task. The implementation details are described later. Next, we will introduce the family of rank based loss functions.

4.1. Pointwise Ranking

In pointwise ranking loss formulation, 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 objec-

Algorithm 1 Gradient-descent implementation of decision-focused learning problems with Ranking Loss

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

```

1: Initialize  $\omega$ 
2: Initialize  $S = \{v^*(c_i) | (x_i, c_i) \in D\}$ 
   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()  $< p_{solve}$  then
7:        $v^*(\hat{c}_i) \leftarrow$  call solver to solve Eq. (1),
8:        $S \leftarrow S \cup \{v^*(\hat{c}_i)\}$ 
9:     end if
10:     $\mathcal{L} += L(\hat{c}_i, c_i; S)$ 
11:  end for
12:   $\omega \leftarrow \omega - \alpha \frac{\partial \mathcal{L}}{\partial \omega}$  # backward pass
13: end for
    
```

tive function value. Thus, we propose the **pointwise loss** function

$$L_P(\hat{c}, c; S) = \frac{1}{|S|} \sum_{v \in S} (f(v, \hat{c}) - f(v, c))^2 \quad (6)$$

that measures the errors in the evaluation of the predicted cost function at each point in S .

Intuitive idea of the pointwise loss function. When the objective function is linear i.e. $f(v, c) = c^\top v$, the pointwise loss (6) becomes

$$L_P(\hat{c}, c; S) = \frac{1}{|S|} \sum_{v \in S} (c^\top v - \hat{c}^\top v)^2 \quad (7)$$

The derivative of this loss is

$$\frac{\partial L_P(\hat{c}, c; S)}{\partial \hat{c}} = -\frac{2}{|S|} \sum_{v \in S} (c^\top v - \hat{c}^\top v) v \quad (8)$$

When considering a combinatorial problem where v is a binary vector, we can see from Eq. (8) that coordinates where v has zeros, will not contribute to the gradient. Moreover, the first component $(c^\top v - \hat{c}^\top v)$ 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:

$$\begin{aligned} L_P(\hat{c}, c; S) &= \sum_{i=1}^K (\hat{c}_i - c_i)^2 \gamma_i + \sum_{i \neq j} (\hat{c}_i - c_i)(\hat{c}_j - c_j) \gamma_{ij} \\ &= \sum_{i=1}^K \epsilon_i^2 \gamma_i + \sum_{i \neq j} \epsilon_i \epsilon_j \gamma_{ij} \end{aligned} \quad (9)$$

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 ϵ_i defined as in (2). In this case, it is a weighted version of the **mse** function plus a term that measures the pairwise relationship of errors of the coordinates.

Moreover, when $V \subseteq \{0, 1\}^K$, the weight γ_i is the frequency of how many times coordinate v_i takes value 1 (since $v_i^2 = v_i$). Coefficients γ_{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 **mse** plus a regularizer which penalizes the crossed-errors between coordinates of the vector c .

4.2. Pairwise Ranking

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 $[2, -5]$. The objective values at these four points are 0, -5 , 2 and -3 , hence $v^*(c) = [0, 1]$. Now let \hat{c}_1 be $[-1, 1]$ and \hat{c}_2 be $[5, -11]$. 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. With this motivation behind, we will construct the pairwise ranking loss function.

Let (p, q) be an ordered pair in S with respect to c . We define OP_c^S 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:

$$(p, q) \in \text{OP}_c^S \implies f(v^p, c) < f(v^q, c) \quad (10)$$

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. In the standard pairwise *margin* ranking loss formulation (Joachims, 2002), the loss is zero, if $f(v^p, \hat{c})$ is smaller than $f(v^q, \hat{c})$ by at least a margin of $\nu > 0$. With this notion of margin, we introduce the following generic **pairwise loss**

$$\begin{aligned} L_{\text{OP}_c^S}(\hat{c}, c) &= \\ \frac{1}{|\text{OP}_c^S|} \sum_{(p, q) \in \text{O.P.}_c^S} \max(0, \nu + f(v^p, \hat{c}) - f(v^q, \hat{c})) \end{aligned} \quad (11)$$

Ordered pairs generation. Eq. (11) is built upon the concept of a pairwise ranking loss (Borges 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 $\mathcal{O}(|S|^2)$. To overcome this implementation challenge, we consider *best-versus-rest* scheme, i.e. $\text{OP}_c^S = \{(v^{p_1}, v^{p_2}), (v^{p_1}, v^{p_3}), \dots, (v^{p_1}, v^{p_S})\}$, where $v^{p_1} = v^*(c)$. With this *best-versus-rest* pair generation scheme and γ being 0, Eq. (11) becomes

$$\frac{1}{|S|} \sum_{v^q \in S} \max(0, (f(v^*(c), \hat{c}) - f(v^q, \hat{c}))) \quad (12)$$

We point out that (12) takes the form of (5), without the *relu* operator. This shows that the NCE approach of Mulamba et al. (2021), although derived differently, can be seen as a special case of our *best-versus-rest* pairwise approach.

Example continued. 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 $\{([0, 1], [1, 1]), ([0, 1], [0, 0]), ([0, 1], [1, 0])\}$. 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 *difference* in objective value. To do so, we propose a loss function over the difference over pairs of solutions their cost vectors \hat{c}_i and c_i . This **pairwise difference loss** function can be formulated as:

$$L_{pd}(\hat{c}, c; S) = \frac{1}{|S|} \sum_{(p,q) \in \text{OP}_c^S} \left((f(v^p, \hat{c}) - f(v^q, \hat{c})) - (f(v^p, c) - f(v^q, c)) \right)^2 \quad (13)$$

For the sake of clarity, we omitted O.P._c^S from the definition of L_{pd} .

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

$$L_{pd}(\hat{c}, c; S) = \sum_{i=1}^K \epsilon_i^2 \bar{\gamma}_i + \sum_{i \neq j} \epsilon_i \epsilon_j \bar{\gamma}_{ij} \quad (14)$$

where $\bar{\gamma}_i = \frac{1}{|S|} \sum_{(p,q)} (v_i^p - v_i^q)^2$, which is proportional to how many times v_i^p and v_i^q are different, and $\bar{\gamma}_{ij} = \frac{1}{|S|} \sum_{(p,q)} (v_i^p - v_i^q)(v_j^p - v_j^q)$. As in the pointwise loss, the pairwise difference loss can be seen as a weighted **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 $\{([0, 1], [1, 1]), ([0, 1], [0, 0]), ([0, 1], [1, 0])\}$. 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 $(2+1)^2 + (5+1)^2 + (7+2)^2 = 94$ and $(2-5)^2 + (5-11)^2 + (7-16)^2 = 94$.

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. Instead of using Eq. (4) directly, we further introduce a temperature parameter τ (Niepert et al., 2021) to define

$$p_\tau(v|c) = \frac{\exp\left(-\frac{f(v,c)}{\tau}\right)}{\sum_{v' \in V} \exp\left(-\frac{f(v',c)}{\tau}\right)} \quad \forall v \in V \quad (15)$$

In this formulation, τ controls the smoothness of the distribution. As $\tau \rightarrow 0$, $p_\tau(v|c)$ takes the form of a categorical distribution with *only* $v^*(c)$ having positive probability mass. As τ increases $p_\tau(v|c)$ converges to a uniform distribution in V .

In order 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 loss is the cross entropy loss between the predicted and the target distribution. Following this idea, we define **listwise loss** as the cross entropy loss between $p_\tau(v|c)$ and $p_\tau(v|\hat{c})$ for all $v \in S$:

$$L_S^l(\hat{c}, c) = -\frac{1}{|S|} \sum_{v \in S} p_\tau(v|c) \log p_\tau(v|\hat{c}) \quad (16)$$

We remark that we could also consider the KL divergence loss instead of cross entropy loss and define listwise loss as

$$\frac{1}{|S|} \sum_{v \in S} p_\tau(v|c) \left(\log p_\tau(v|c) - \log p_\tau(v|\hat{c}) \right)$$

Using this loss formulation, we obtained similar results to Eq.(16) and do not further discuss it.

4.5. Implementation

So far we define pointwise (6) pairwise (11), pairwise-difference (13) and listwise (16) ranking losses. As mentioned, the fundamentals of the LTR loss functions is to

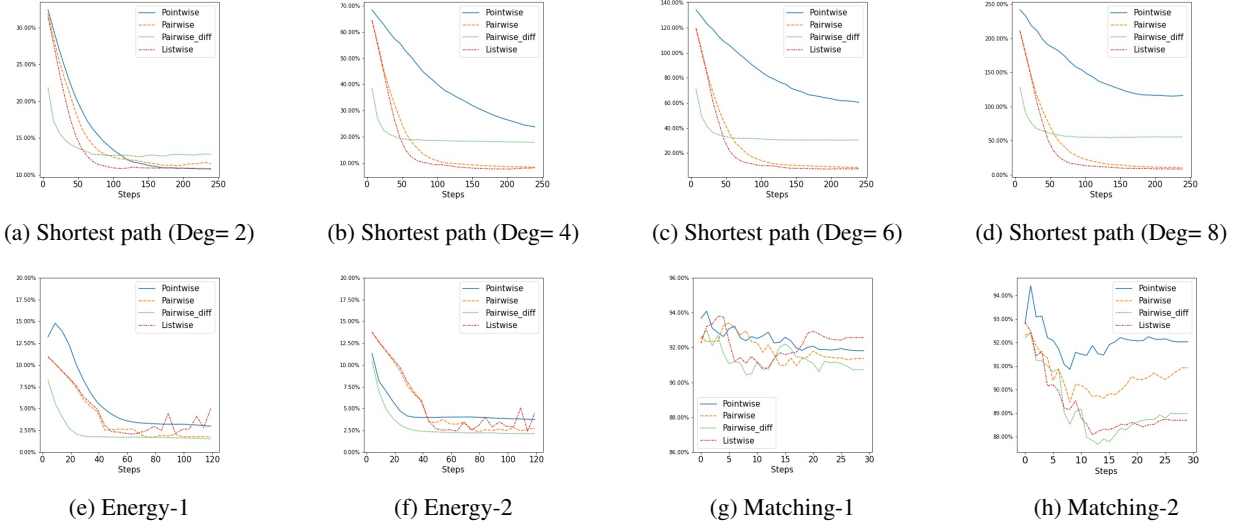


Figure 1. Learning Curve. We show how the average regrets on validation dataset progress as the models learn.

learn the partial ordering of $v \in S$. To construct and expand S , we use the strategy of [Mulamba et al. \(2021\)](#). The generic structure of the proposed algorithm is shown in Algorithm 1, which is a modified version of standard gradient descent algorithms for decision-focused learning problems. They proposed to initialise S with all true optimal solutions. In Algorithm 1 S is initialized by caching all the optimal solutions of the training instances in line 2. To expand S , they defined a hyperparameter p_{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 . This is demonstrated in line 8 in Algorithm 1. Obviously with $p_{solve} = 100\%$, Eq. (1) is solved for every \hat{c}_i during training.

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. The part that can not be run on GPU is calling an optimization oracle to expand S .

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 & Grigas \(2021\)](#). It is a shortest path problem in a 5×5 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. They generate the cost vector as per the following model

$$c_{ij} = \left(\frac{1}{\sqrt{p}} (Bx_i) + 3 \right)^{\text{Deg}} \epsilon_i^j \quad (17)$$

where c_{ij} is the j -th component of cost vector c_i and B is the latent data generation matrix. Deg specifies the extent of model specification, the higher the value of Deg, the more it deviates from a linear model and the more errors there will be. We experiment with degree of 1, 2, 4, 6 and 8. ϵ_i^j is a multiplicative noise that is sampled from $U(0.5, 1.5)$. For each degree, we have 1000, 250 and 10,000 training, validation and test instances¹. 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 & Walsh, 1999](#)), a library of constraint optimization problems. In energy-cost aware scheduling ([Simonis et al., 1999](#)), a given number of tasks, to be scheduled on a certain number of machines without violating the resource capacities of each machine. The goal of the optimization problem is to find the scheduling which would minimize the total energy consumption subject to the energy prices, which would be realized 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, forecasted energy-load, wind-energy production and prices. We take the energy price data from [Ifrim](#)

¹The dataset is generated as described in <https://github.com/paulgrigas/SmartPredictThenOptimize>

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

	Pointwise	Pairwise	Pairwise-diff	Listwise	NCE	MAP	SPO	Blackbox	Twostage
Shortest Path Problem									
Deg-1	15.45%	16.37%	16.00%	15.56%	23.63%	19.68%	15.51%	18.62%	15.45%
Deg-2	10.07%	10.74%	11.60%	10.41%	30.84%	14.15%	10.06%	13.26%	10.07%
Deg-4	19.27%	8.06%	17.89%	7.71%	65.10%	9.44%	7.98%	9.39%	10.44%
Deg-6	72.18%	9.27%	32.63%	8.29%	129.42%	9.45%	16.19%	9.69%	15.96%
Deg-8	178.16%	12.75%	61.80%	12.38%	242.30%	13.68%	33.75%	14.14%	28.50%
Energy Scheduling Problem									
Energy-1	2.51%	1.65%	1.63%	1.67%	1.69%	1.59%	1.56%	1.54%	1.91%
Energy-2	2.83%	2.08%	2.04%	1.96%	2.23%	2.01%	1.93%	1.93%	2.46%
Bipartite Matching Problem									
Matching-1	90.17%	88.80%	88.23%	88.49%	89.39%	89.13%	88.70%	90.09%	90.12%
Matching-2	89.86%	87.24%	85.87%	86.40%	85.31%	84.80%	85.79%	90.31%	89.42%

et al. (2012). 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.

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 the rank based loss functions. As described in section 4, we train the neural network with respect to these loss functions². As our objective is to have lower regret, we consider the percentage regret ($\frac{f(v^*(\hat{c}), c) - f(v^*(c), c)}{f(v^*(c), c)}$) as the evaluation metric. One way to know whether model training decreases the regret is to monitor the regret on the validation dataset. Figure 1 validates that by minimizing the surrogate losses, the neural network models learn to lower the regret. In the shortest path problem, overall, the listwise and pairwise loss func-

tions perform better than the other two. The difference is more pronounced in higher degrees, where the linear model makes larger error. In the scheduling and matching experiments, the pairwise difference loss generalizes the best. The lowest regret of listwise loss is similar to pairwise difference, but its learning curve is less stable.

Next we compare the rank based loss functions with the SPO+ loss (Elmachtoub & Grigas, 2021), Blackbox back-propagation approach (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. We present average regret on test data of 10 independent trials in Table 1. We refer the readers to C to view the distribution of the regrets. For the shortest path problem, we again 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 4, 6 and 8, the listwise loss function produces the lowest regret. For lower two degrees, the pointwise and pairwise difference loss function produces low regret, but their regret jumps up at higher degrees. This is reasonable as their loss functions include the absolute difference between the predicted and true solutions. Listwise loss comes second among all in Energy-2 and Matching-1. The pairwise difference loss has lowest regret in Matching-1 and its regret is competitive with the best loss function in these two problems. 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. Overall, Table 1 and Figure 1 indicate the performance of the pairwise difference loss is steady when the underlying predictive model is consistent with the data generation process, whereas the listwise loss is robust and reliable across all problem instances.

²The code is available at <https://github.com/JayMan91/ltr-predopt>.

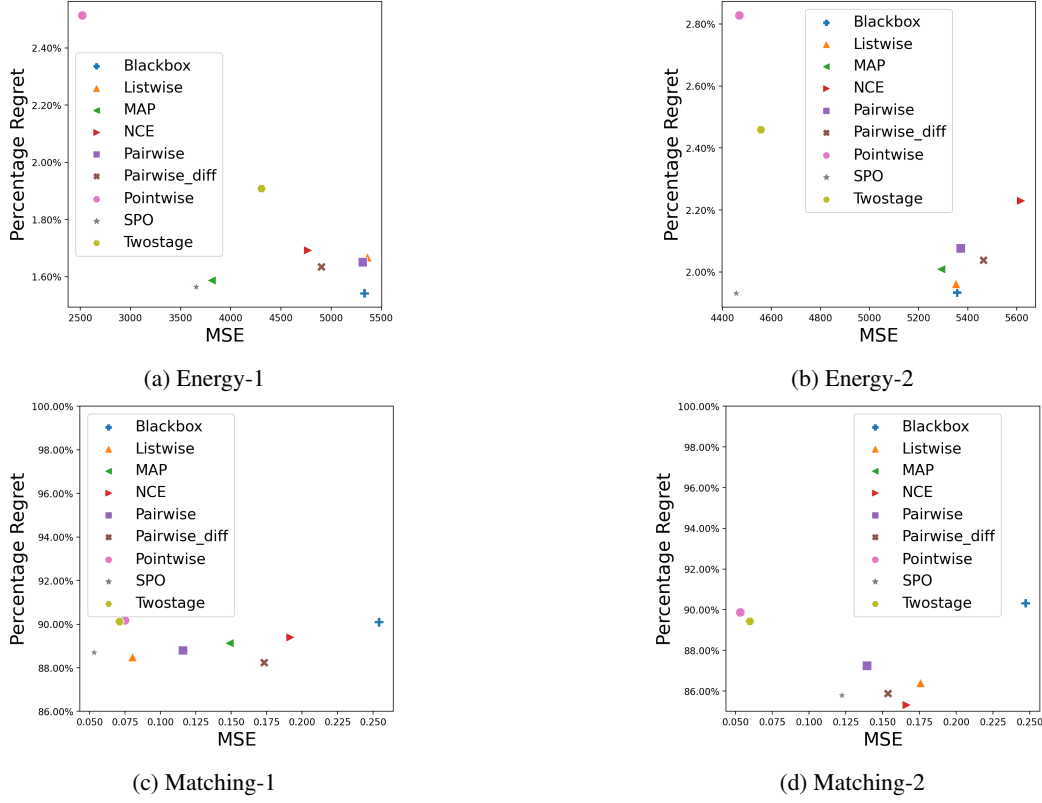


Figure 2. MSE vs Regret trade-off

 Table 2. Impact of p_{solve} on per epoch training time and regret in Energy scheduling instances

	p_{solve}	Pointwise		Pairwise		Pairwise-diff		Listwise	
		Regret	Time (s)	Regret	Time (s)	Regret	Time (s)	Regret	Time (s)
Energy-1	100%	2.12%	110	1.64%	110	1.63%	110	1.72%	100
	10%	2.51%	30	1.65%	30	1.61%	30	1.67%	25
Energy-2	100%	2.70%	130	2.05%	140	2.07%	140	1.99%	120
	10%	2.83%	40	2.08%	45	2.04%	45	1.96%	40

MSE vs Regret tradeoff. 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. 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 very low, comparable to minimizing MSE. 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 art in terms of regret, their MSE loss remains high. In this experiment we will consider a convex combination of MSE loss and listwise ranking loss, inspired by (Sculley, 2010) but formulated as a multi-task problem instead of sampling between the two losses:

$$\alpha L_S^l(\hat{c}, c) + (1 - \alpha) \text{mse}(\hat{c}, c) \quad (18)$$

The motivation behind this loss function is that we can control α as a tuning parameter. Clearly, $\alpha = 0$ results in MSE loss whereas $\alpha = 1$ results in listwise ranking loss. Figure 3 displays the impact α on the two scheduling instances. As hypothesised, we see MSE goes up and regret goes down as we increase α . This experiment suggests it is possible to choose a value of α so that we sacrifice regret (problem-specific) to attain predictions with lower MSE (close to the true values).

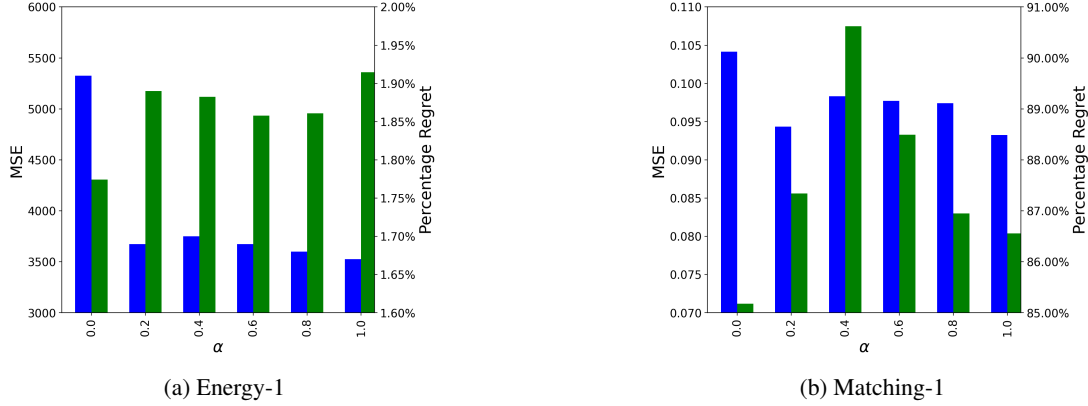


Figure 3. Change of MSE and Regret with α as a tuning parameter. The green and blue bar present the MSE loss and percentage regret respectively.

Impact of p_{solve} . The motivation behind ours (and [Mulamba et al. \(2021\)](#)) approach is reducing the number of times of the optimization problem is solved during training. In the next experiment, we show how p_{solve} impacts the model training time. Lower values of p_{solve} 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 $p_{solve} = 10\%$ 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_{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 extend the approach of [Mulamba et al. \(2021\)](#), which introduces surrogate loss functions for decision-focused learning problems by caching a subset of feasible solutions. Motivated by their work, we frame the decision-focused learning problem as a learning to rank problem, where we train models to learn the partial ordering of the pool of feasible solutions. This generalizes their approach and inherits its nice properties of separating the solving from the loss computation. We also attempt 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 decision-focused learning.

Acknowledgements

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A. Problem Specification

A.1. Shortest Path Problem

In this problem, we consider shortest path problem on 5×5 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.

$$\begin{aligned} \min_{x \geq 0} \quad & c^\top x \\ \text{subject to} \quad & Ax = b \end{aligned}$$

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 e_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:

$$\begin{aligned} \min_{x_{jmt}} \quad & \sum_{j \in J} \sum_{m \in M} \sum_{t \in T} x_{jmt} \left(\sum_{t \leq t' < t + d_j} p_j c_{t'} \right) \\ \text{subject to} \quad & \sum_{m \in M} \sum_{t \in T} x_{jmt} = 1, \forall j \in J \\ & x_{jmt} = 0 \quad \forall j \in J \forall m \in M \forall t < e_j \\ & x_{jmt} = 0 \quad \forall j \in J \forall m \in M \forall t + d_j > l_j \\ & \sum_{j \in J} \sum_{t - d_j < t' \leq t} x_{jmt'} u_{jr} \leq c_{mr}, \forall m \in M \forall r \in R \forall t \in T \end{aligned}$$

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 $m_{i,j}$ is 0 if article i and 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:

$$\begin{aligned} \max_x \quad & \sum_{i,j} c_{i,j} x_{i,j} \\ \text{subject to} \quad & \sum_j x_{i,j} \leq 1 \quad \forall i \in N_1 \\ & \sum_i x_{i,j} \leq 1 \quad \forall j \in N_2 \\ & \sum_{i,j} m_{i,j} x_{i,j} \geq p \sum_{i,j} x_{i,j} \\ & \sum_{i,j} (1 - m_{i,j}) x_{i,j} \geq q \sum_{i,j} x_{i,j} \\ & x_{i,j} \in \{0, 1\} \quad \forall i \in N_1, j \in N_2 \end{aligned}$$

In our experiments, we considered two variations of this problem with $p = q =$ being 25% and 5%, respectively named Matching-1 and Matching-2.

B. Hyperparameter Configuration

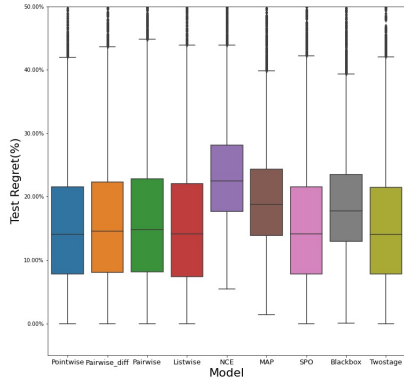
To reproduce the result reported in this paper use the hyperparameter settings as described in Table 3.

Table 3. Details of hyperparameters for reproducing the result

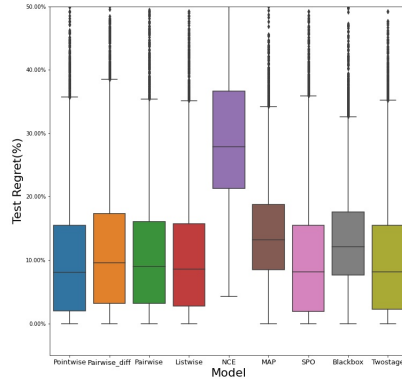
		Shortest Path Problem				
		Deg-1	Deg-2	Deg-4	Deg-6	Deg-8
Pointwise	learning rate	0.8	0.8	0.8	0.8	0.8
Pairwise	learning rate	0.1	0.1	0.1	0.1	0.1
	margin	1.0	0.1	0.1	0.1	0.1
Listwise	learning rate	0.1	0.1	0.1	0.1	0.1
	temperature	1.0	0.1	0.05	0.05	0.05
Pairwise-difference	learning rate	0.1	0.1	0.1	0.5	0.5
NCE	learning rate	0.5	0.5	0.5	0.5	0.5
MAP	learning rate	0.05	0.05	0.05	0.7	0.7
SPO	learning rate	0.1	0.5	0.5	0.5	0.1
Blackbox	learning rate	0.5	0.5	0.5	0.5	0.5
	displace parameter	1.	1.	1.	1.	1.
Twostage	learning rate	0.5	0.5	0.1	0.5	0.5
		Energy Scheduling		Bipartite Matching		
		Energy-1	Energy-2	Matching-1	Matching-2	
Pointwise	learning rate	0.9	0.5	0.01	0.01	
Pairwise	learning rate	0.1	0.1	0.001	0.01	
	margin	100	100	0.2	1.0	
Listwise	learning rate	0.1	0.1	0.005	0.01	
	temperature	1.0	1.0	0.01	1.0	
Pairwise-difference	learning rate	0.5	0.5	0.01	0.01	
NCE	learning rate	0.5	0.5	0.001	0.01	
MAP	learning rate	0.5	0.5	0.001	0.01	
SPO	learning rate	0.9	0.9	0.01	0.01	
Blackbox	learning rate	0.1	0.1	0.01	0.01	
	displace parameter	0.001	0.1	10^{-5}	0.001	
Twostage	learning rate	0.7	0.7	0.01	0.01	

C. Distribution of the regret of the predictions

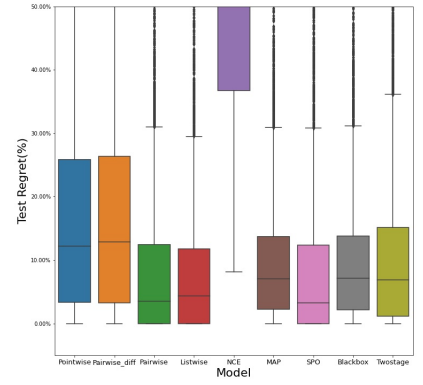
In Table 1, we report only the average regret of all the instances over 10 independent trails. In Figure fig:boxplot, we show the distributions of the regret across all the test instances with box-plots for the three problems.



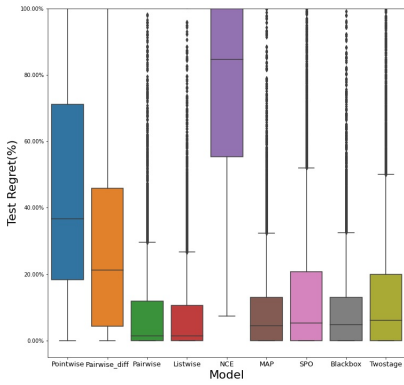
(a) Shortest path (Deg= 1)



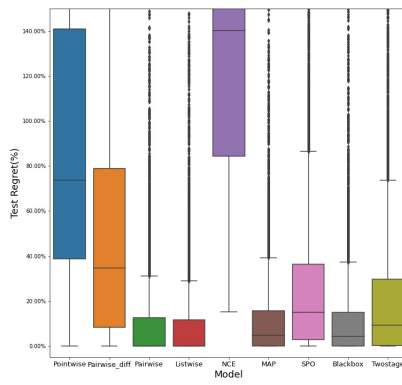
(b) Shortest path (Deg= 2)



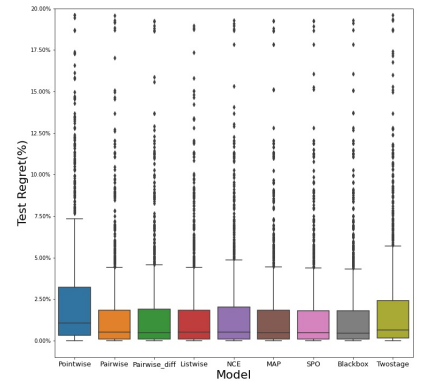
(c) Shortest path (Deg= 4)



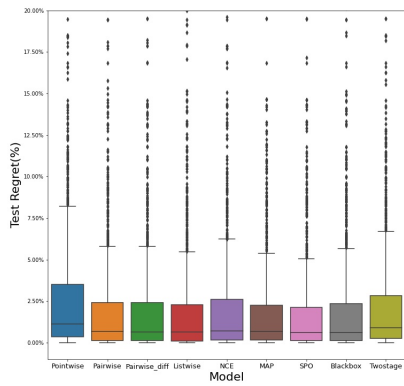
(d) Shortest path (Deg= 6)



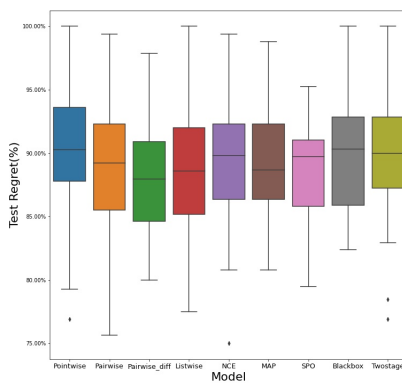
(e) Shortest path (Deg= 8)



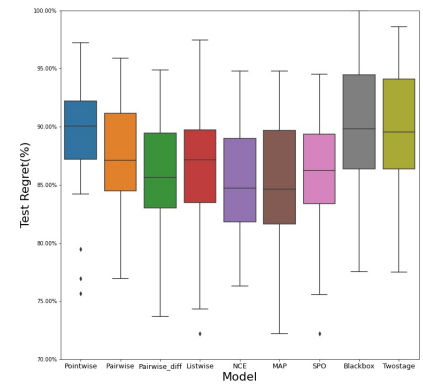
(f) Energy-1



(g) Energy-2



(h) Matching-1



(i) Matching-2

Figure 4. Boxplot