PyEPO: A PyTorch-based End-to-End Predict-then-Optimize Library for Linear and Integer Programming

Bo Tang · Elias B. Khalil

Received: date / Accepted: date

Abstract In deterministic optimization, it is typically assumed that all problem parameters are fixed and known. In practice, however, some parameters may be a priori unknown but can be estimated from historical data. A typical predict-then-optimize approach separates predictions and optimization into two stages. Recently, end-to-end predict-then-optimize has become an attractive alternative. In this work, we present the PyEPO package, a PyTorch-based end-to-end predict-then-optimize library in Python. To the best of our knowledge, PyEPO (pronounced like pineapple with a silent “n”) is the first such generic tool for linear and integer programming with predicted objective function coefficients. It provides four base algorithms: a convex surrogate loss function from the seminal work of Elmachtoub and Grigas [16], a differentiable black-box solver approach of Poganˇc´ic et al. [35], and two differentiable perturbation-based methods from Berthet et al. [6]. PyEPO provides a simple interface for the definition of new optimization problems, the implementation of state-of-the-art predict-then-optimize training algorithms, the use of custom neural network architectures, and the comparison of end-to-end approaches with the two-stage approach. PyEPO enables us to conduct a comprehensive set of experiments comparing a number of end-to-end and two-stage approaches along axes such as prediction accuracy, decision quality, and running time on problems such as Shortest Path, Multiple Knapsack, and the Traveling Salesperson Problem. We discuss some empirical insights from
these experiments, which could guide future research. PyEPO and its documentation are available at [https://github.com/khalil-research/PyEPO](https://github.com/khalil-research/PyEPO).

**Keywords** Data-driven optimization · Mixed integer programming · Machine learning

**Mathematics Subject Classification (2020)** 90-04, 90C11, 62J05

1 Introduction

Predictive modeling is ubiquitous in real-world decision-making. For instance, in many applications, the objective function coefficients of the optimization problem, such as travel time in a routing problem, customer demand in a delivery problem, and assets return in portfolio optimization, are unknown at the time of decision-making. In this work, we are interested in the commonly used paradigm of prediction followed by optimization in the context of linear programs or integer linear programs, two widely applicable modeling frameworks. Here, it is assumed that a set of features describe an instance of the optimization problem. A regression model maps the features to the (unknown) objective function coefficients. A deterministic optimization problem is then solved to obtain a solution. Due to its wide applicability and simplicity compared to other frameworks for optimization under uncertain parameters, the predict-then-optimize paradigm has received increasing attention in recent years.

One natural idea is to proceed in two stages, first training an accurate predictive model, then solving the downstream optimization problem using predicted coefficients. However, prediction errors such as mean squared error cannot measure the quality of decisions appropriately. While a perfect prediction would always yield an optimal decision, learning a prediction model without errors is impracticable. Bengio [5], Ford et al. [19], and Elmachtoub and Grigas [16] reported that training a predictive model based on prediction error leads to worse decisions than directly considering decision error. Thus, the state-of-art alternative is to integrate optimization into prediction, taking into account the impact on the decision – the so-called end-to-end learning framework.

End-to-end predict-then-optimize requires embedding an optimization solver into the model training loop. Classical solution approaches for linear and integer linear models, including graph algorithms, linear programming, integer programming, constraint programming, etc., are well-established and efficient in practice. In addition, commercial solvers such as Gurobi [22] and CPLEX [9] are highly optimized and enable users to easily express business or academic problems as optimization models without a deep understanding of theory and algorithms. However, embedding a solver for end-to-end learning requires additional computation and integration (e.g., gradient calculation) that current software does not provide.
On the other hand, the field of machine learning has witnessed tremendous growth in recent decades. In particular, breakthroughs in deep learning have led to remarkable improvements in several complex tasks. As a result, neural networks now pervade disparate applications spanning computer vision, natural language, and planning, among others. Python-based machine learning frameworks such as Scikit-Learn [34], TensorFlow [1], PyTorch [33], MXNet [8], etc., have been developed and extensively used for research and production needs. Although deep learning has proven highly effective in regression and classification, it lacks the ability to handle constrained optimization such as integer linear programming.

Since Amos and Kolter [4] first introduced a neural network layer for generic mathematical optimization, there have been some prominent attempts to bridge the gap between optimization solvers and the deep learning framework. The critical component is typically a differentiable block for optimization tasks. With a differentiable optimizer or a direct decision loss function, neural network packages enable the computation of gradients for optimization operations and then update predictive model parameters based on a loss function that depends on decision quality.

While research code implementing a number of predict-then-optimize training algorithms have been made available for particular classes of optimization problems and/or predictive models [21, 14, 36, 17, 25, 55, 26, 12, 3, 2], there is a dire need for a generic end-to-end learning framework, especially for linear and integer programming. In this paper, we propose the open-source software package PyEPO which aims to customize and train end-to-end predict-then-optimize for linear and integer programming. Our contributions are as follows:

1. We implement SPO+ (“Smart Predict-then-Optimize+”) loss [16], DBB (differentiable black-box) solver [35], DPO (differentiable perturbed optimizer), and PFYL (perturbed Fenchel-Young loss), which are four typical end-to-end methods for linear and integer programming.
2. We build PyEPO based on PyTorch. As one of the most popular deep learning frameworks, PyTorch makes it easy to use and integrate any deep neural network.
3. We provide interfaces to the Python-based optimization modeling frameworks GurobiPy and Pyomo. Such high-level modeling languages allow non-specialists to formulate optimization models with PyEPO.
4. We enable parallel computing for the forward pass and backward pass in PyEPO. Optimizations in training are carried out in parallel, allowing users to harness multiple processors to reduce training time.
5. We present new benchmark datasets for end-to-end predict-then-optimize, allowing us to compare the performance of different approaches.
6. We conduct and analyze a comprehensive set of experiments for end-to-end predict-then-optimize. We compare the performance of different methods on a number of datasets. We show the competitiveness of end-to-end learning and the surprising effect of relaxations and hyperparameter tuning. A
number of empirical findings are reported to support new research directions within this topic.

2 Related work

In early work on the topic, Bengio [5] introduced a differentiable portfolio optimizer and suggested that direct optimization with financial criteria has better performance in neural networks compared to the mean squared error of predicted values. Kao et al. [25] trained a linear regressor with a convex combination of prediction error and decision error, but they only considered unconstrained quadratic programming. With the success of deep learning, predict-then-optimize research has adopted gradient-based methods. Donke [13] investigated generic gradient-descend methods to minimize unconstrained energy functions. More recently, the interest has been in constrained optimization problems that represent much of the real-world applications. For instance, Gould et al. [21] allows differentiating bi-level optimization problems with and without constraints. In subsequent studies, a comprehensive exploration of differentiable constraint optimization encompasses various types of optimization problems such as quadratic programming, linear programming, and integer linear programming. A comparison of methodologies for end-to-end constrained optimization are presented in Table 1 and Table 2. Another notable piece of work that does not employ gradients is that of the predict-then-optimize decision tree of Elmachtoub et al. [15].

2.1 Gradients of Optimal Solutions via the KKT Conditions

Gradient-based end-to-end learning requires well-defined first-order derivatives of an optimal solution with respect to the cost vector. The KKT conditions become an attractive option because they make the optimization problem with hard constraints differentiable.

Amos and Kolter [4] proposed OptNet, which derives gradients of constrained quadratic programs from the KKT conditions. Based on OptNet, Donti et al. [14] investigated a general end-to-end framework, DQP, for learning with constrained quadratic programming, which improved decision-making over two-stage models. Although linear programming is a special case of quadratic programming, DQP has no ability to tackle linear objective functions because the gradient is zero almost everywhere and undefined otherwise.

Nevertheless, Amos and Kolter [4] adopted a quadratic objective for the Sudoku problem, effectively expressing a linear constraint satisfaction problem as a quadratic problem to obtain useful gradients. Similarly, Wilder et al. [36] take inspiration from OptNet and add a small quadratic objective term on DQP to make a linear program second-order differentiable, resulting in QPTL. Wilder et al. [36] also discussed the relaxation and rounding for the approximation of binary problems. Further, Ferber et al. [17] followed up on QPTL with
**MIPaal**, a cutting-plane approach to support (mixed) integer programming. With the cutting-plane method, MIPaal generates (potentially exponentially many) valid cuts to convert a discrete problem into an equivalent continuous problem, which is theoretically sound for combinatorial optimization but extremely time-consuming. In addition, Mandi and Guns [26] introduced IntOpt based on the interior-point method, which computes gradients for linear programming with log-barrier term instead of the quadratic term of the QPTL. Except for MIPaal [17], end-to-end learning approaches for (mixed) integer programming use linear relaxation during training but evaluate with optimal integer solutions at test time.

Besides DQP and its extension, Agrawal et al. [2] introduced a generic framework, CvxpyLayers, which differentiates through the KKT conditions of the conic program. The central idea in CvxpyLayers is to canonicalize disciplined convex programming as conic programming so that it is applicable to a wider range of convex optimization problems. In particular, for problems such as linear programs which cannot be differentiated at a solution, a least-squares solution is used as a heuristic.

However, these KKT-based methods require a solver for either quadratic or conic programming. Linear programming requires additional objective terms and the solver efficiency of the above implementations is not comparable to commercial MILP solvers such as Gurobi [22] and CPLEX [9]. Furthermore, they do not naturally support discrete optimization due to non-convexity.

| Method      | In PyEPO | w/ Unk Constr | Disc Var | Lin Obj | Quad Obj |
|-------------|----------|---------------|----------|---------|----------|
| DQP [14]    | X        | ✓             | ✓        | ✓       | ✓        |
| QPTL [36]   | [code]   | ✓             | ✓        | ✓       | ✓        |
| MIPaal [17] | X        | ✓             | ✓        | ✓       | ✓        |
| IntOpt [26] | [code]   | ✓             | ✓        | ✓       | ✓        |
| CvxpyLayers [2] [code] | ✓ | ✓ | ✓ | ✓ | ✓ |
| SPO+ [16]   | [code]   | ✓             | ✓        | ✓       | ✓        |
| SPO+ Rel [27] [code] | ✓ | ✓ | ✓ | ✓ | ✓ |
| SPO+ WS [27] [code] | ✓ | ✓ | ✓ | ✓ | ✓ |
| DBB [35]    | [code]   | ✓             | ✓        | ✓       | ✓        |
| DPS [6]     | [code]   | ✓             | ✓        | ✓       | ✓        |
| PFYL [6]    | [code]   | ✓             | ✓        | ✓       | ✓        |

Table 1: Methodology Comparison
This is a comparison diagram for different methodologies. The first set of methods uses the KKT conditions, and the second part is based on differentiable approximations.

"In PyEPO" denotes whether the method is available in PyEPO.
"w/ Unk Constr" denotes whether unknown parameters occur in constraints.
"Disc Var" denotes whether the method supports integer variables.
"Lin Obj" denotes whether the method supports a linear objective function.
"Quad Obj" denotes whether the method supports a quadratic objective function.
2.2 Differentiable Approximations as an Alternative to KKT

Since the KKT conditions may not be ideal for linear programming, researchers have also explored designing gradient approximations. For example, Elmachtoub and Grigas [16] proposed regret (SPO loss in their paper) to measure decision error. Since the regret loss suffers from non-convexity and discontinuity of linear programming, they then developed a method SPO+, in which a convex and sub-differentiable loss guaranteed that a useful subgradient could be computed and used to guide training. Same as previous approaches, SPO+ solves an optimization problem in each forward pass. In contrast to the KKT-based methods, SPO+ is limited to the linear objective function. Because optimization is the computational bottleneck of SPO+, Mandi et al. [27] utilized SPO+ on combinatorial problems by applying a relaxation as well as warm starting. As Mandi et al. [27] reported, the usage of a relaxation reduced the solving time at the cost of performance.

On the other hand, Pogančić et al. [35] computed a subgradient from continuous interpolation of linear objective functions, an approach they referred to as the “differentiable black-box solver”, DBB. The interpolation approximation was non-convex but also avoided vanishing gradients. Compared to SPO+, DBB requires an extra optimization problem for the backward pass, and the loss of DBB is flexible (the Hamming distance in their paper). In addition, Berthet et al. [6] applied perturbed optimizer DPO by adding random noise to the cost vector so that a nonzero expected derivative of linear programming can be obtained and further constructed Fenchel-Young loss PFYL. As the key algorithms of PyEPO, SPO+, DBB, DPO, and PFYL are further discussed in Section 3.

2.3 Software for Predict-then-Optimize

Research code. Table 1 lists and links to the codebases that will be discussed next. Amos and Kolter [4] developed a PyTorch-based solver qpth for OptNet, which was used to solve a quadratic program and compute its derivatives efficiently. The solver was based on an efficient primal-dual interior-point method [29] and can solve batches of quadratic programs on a GPU. Using this solver, Donti et al. [14] provided an open-source repository to reproduce the DQP experiments; the repository was specifically designed for inventory, power scheduling, and battery storage problems. Wilder et al. [36] provided code for QPTL for budget allocation, bipartite matching, and diverse recommendation. MIPaaS [17] relied on qpth and used CPLEX to generate cutting planes, but there is no available open-source code. Mandi and Guns [26] released InOpt code for knapsack, shortest path, and power scheduling, Berthet et al. [6] contributed the TensorFlow-based DPO and PFYL implementation, which provided universal functions for end-to-end predict-then-optimize but required users to create additional helper methods for tensor operations. Other approaches, including SPO+ [16, 27] and DBB [35], have open-source code. Elmachtoub and
Grigas [16] provided an implementation of SPO+ in Julia, which contained the shortest path and portfolio optimization problems, while Mandi et al. [27] implemented SPO+ with Python for the knapsack and power scheduling problems. Code for DBB [35] as applied to shortest path, traveling salesperson, ranking, perfect matching, and graph matching are available.

Except for DPO and PFYL, the above contributions provided solutions to specific optimization problems, and Berthet et al. [6] did not wrap up DPO and PFYL as a generic library. In conclusion, they were confined to research-grade code for purposes of reproducibility.

Software packages. CvxpyLayers [2] is the first generic end-to-end predict-then-optimize learning framework. In contrast to the above codes, it requires modeling with a domain-specific language CVXPY, which is embedded into a differentiable layer in a straightforward way. The emergence of CvxpyLayers provides a more powerful tool for academia and industry. However, the solver of CvxpyLayers cannot compete with commercial solvers on efficiency, especially for linear and integer linear programming. Since end-to-end training requires repeated optimization in each iteration, the inefficiency of the solver becomes a bottleneck. In addition, the nature of CvxpyLayers means that it cannot support training with integer variables, which limits applicability to many real-world decision-making problems.

| Method       | Computation per Gradient                                                                 |
|--------------|------------------------------------------------------------------------------------------|
| DQP [14]     | GPU-based primal-dual interior-point method for quadratic programming                      |
| QPTL [36]    | GPU-based primal-dual interior-point method for quadratic programming                      |
| MIPaaL [17]  | Cutting-plane method + GPU-based primal-dual interior-point method for quadratic programming |
| IntOpt [26]  | GPU-based primal-dual interior-point method for conic programming                         |
| CvxpyLayers  | GPU-based primal-dual interior-point method for conic programming                         |
| SPO+ [16]    | Linear/integer programming                                                                |
| SPO+ Rel     | Integer programming with warm starting                                                   |
| SPO+ WS [27] | Two Linear/integer programming solves                                                     |
| DPO [6]      | Monte-Carlo sampling, multiple linear/integer programming solves with random noise       |
| PFYL [6]     | Monte-Carlo sampling, multiple linear/integer programming solves with random noise        |

Table 2: Computational cost per gradient calculation for different methodologies.

3 Preliminaries

3.1 Definitions and Notation

For the sake of convenience, we define the following linear programming problem without loss of generality, where the decision variables are \( w \in \mathbb{R}^d \) and all \( w_i \geq 0 \), the cost coefficients are \( c \in \mathbb{R}^d \), the constraint coefficients are
A ∈ R^{k×d}, and the right-hand sides of the constraints are \( b \in R^k \):

\[
\begin{align*}
\min_{w} & \quad c^T w \\
\text{s.t.} & \quad Aw \leq b \\
& \quad w \geq 0
\end{align*}
\]

(1)

When some variables \( w_i \) are restricted to be integers, we obtain a (mixed) integer program:

\[
\begin{align*}
\min_{w} & \quad c^T w \\
\text{s.t.} & \quad Aw \leq b \\
& \quad w \geq 0 \\
& \quad w_i \in \mathbb{Z} \quad \forall i \in D', \quad D' \subseteq \{1, 2, ..., d\}
\end{align*}
\]

(2)

For both linear and integer programming, let \( S \) be the feasible region, \( z^*(c) \) be the optimal objective value with respect to cost vector \( c \), and \( w^*(c) \in W^*(c) \) be a particular optimal solution derived from some solver. We define the optimal solution set \( W^*(c) \) because there may be multiple optima.

As mentioned before, some coefficients are unknown and must be predicted before optimizing. Here we assume that only the cost coefficients of the objective function \( c \) are unknown, but they correlate with a feature vector \( x \in \mathbb{R}^p \). Given a training dataset \( D = \{(x_1, c_1), (x_2, c_2), ..., (x_n, c_n)\} \) or \( D = \{(x_1, w^*(c_1)), (x_2, w^*(c_2)), ..., w^*(x_n, c_n)\} \), one can train a machine learning predictor \( g(·) \) to minimize a loss function \( l(·) \), where \( \theta \) is the vector of predictor parameters and \( \hat{c} = g(x; \theta) \) is the prediction of the cost coefficient vector \( c \).

3.2 The Two-Stage Method

As Figure 1 shows, the two-stage approach trains a predictor \( g(·) \) by minimizing a loss function w.r.t. the true cost vector \( c \) such as mean squared error (MSE), \( l_{\text{MSE}}(\hat{c}, c) = \frac{1}{n} \| \hat{c} - c \|^2 \). Following training, and given an instance with feature vector \( x \), the predictor outputs a cost vector \( \hat{c} = g(x; \theta) \), which is then used for solving the optimization problem. The advantage of the two-stage approach is the utilization of existing machine learning methods. It decomposes the predict-then-optimize problem into a traditional regression and then an optimization.

3.3 Gradient-based End-to-end Predict-then-Optimize

The main drawbacks of the two-stage approach are that the decision error is not taken into account in training, and the prediction of costs requires true costs as labels. In contrast, the end-to-end predict-then-optimize method in Figure 2 attempts to minimize the decision error and has the potential
Fig. 1: Illustration of the two-stage predict-then-optimize framework: A labeled dataset $\mathcal{D}$ of $(x, c)$ pairs is used to fit a machine learning predictor that minimizes prediction error. At test time (grey box), the predictor is used to estimate the parameters of an optimization problem, which is then tackled with an optimization solver. The two stages are thus completely separate.

Fig. 2: Illustration of the end-to-end predict-then-optimize framework: A labeled dataset $\mathcal{D}$ of $(x, c)$ or $(x, w^*(c))$ pairs is used to fit a machine learning predictor that directly minimizes decision error. The critical component is an optimization solver which is embedded into a differentiable predictor (e.g., a neural network). At test time, this approach is similar to the two-stage approach from Figure 1.

to learn without true costs. Consistent with deep learning terminology, we will use the term “backward pass” to refer to the gradient computation via the backpropagation algorithm. In order to incorporate optimization into the prediction, we can derive the derivative of the optimization task and then apply the gradient descent algorithm, Algorithm 1, to update the parameters of the predictor.
Algorithm 1 End-to-end Gradient Descent

**Require:** coefficient matrix $A$, right-hand side $b$, data $D$

1: Initialize predictor parameters $\theta$ for predictor $g(x; \theta)$

2: for epochs do
3:     for each batch of training data $(x, c)$ do
4:         Sample batch of the cost vectors $c$ with the corresponding features $x$
5:         Predict cost using predictor $\hat{c} := g(x; \theta)$
6:         Forward pass to compute optimal solution $w^* := \text{argmin}_{w \in S} \hat{c}^T w$
7:         Forward pass to compute decision loss $l(\hat{c}, \cdot)$
8:         Backward pass from loss $l(\hat{c}, \cdot)$ to update parameters $\theta$ with gradient
9:     end for
10: end for

For an appropriately defined loss function, i.e., one that penalizes decision error, the chain rule can be used to calculate the following gradient of the loss w.r.t. predictor parameters:

\[
\frac{\partial l(\hat{c}, \cdot)}{\partial \theta} = \frac{\partial l(\hat{c}, \cdot)}{\partial \hat{c}} \frac{\partial \hat{c}}{\partial \theta} = \frac{\partial l(\hat{c}, \cdot)}{\partial \hat{c}} \frac{\partial w^*(\hat{c})}{\partial \hat{c}} \frac{\partial \hat{c}}{\partial \theta}
\]

\[\text{Note: } \frac{\partial \hat{c}}{\partial \theta} = \frac{\partial g(x; \theta)}{\partial \theta} \tag{3}\]

The last term $\frac{\partial \hat{c}}{\partial \theta}$ is the gradient of the predictions w.r.t. the model parameters, which is trivial to calculate in modern deep learning frameworks. The challenging part is to compute the gradient of a differentiable optimizer $\frac{\partial w^*(\hat{c})}{\partial \hat{c}}$ or the direct decision loss function $\frac{\partial l(\hat{c}, \cdot)}{\partial \hat{c}}$. Because the optimal solution $w^*(c)$ for linear and integer programming is a piecewise constant function from cost vector $c$ to solution vector $w^*$, the predictor parameters cannot be updated with gradient descent. Thus, SPO+ and PYFL, as direct decision loss functions, derive surrogate $\frac{\partial l(\hat{c}, \cdot)}{\partial \hat{c}}$, measuring decision errors with respect to specific losses, while DBB and DPO, as differentiable optimizers, compute approximate $\frac{\partial w^*(\hat{c})}{\partial \hat{c}}$, allowing customized loss functions.

### 3.3.1 Decision Loss

To measure the error in decision-making, the notion of regret (also called SPO Loss [16]) has been proposed and is defined as the difference in objective value between an optimal solution (using the true but unknown cost vector) and one obtained using the predicted cost vector:

\[
l_{\text{Regret}}(\hat{c}, c) = c^T w^*(\hat{c}) - z^*(c) \tag{4}\]

Given a cost vector $\hat{c}$, there may be multiple optimal solutions to $\min_{w \in S} c^T w$. Therefore, Elmachtoub and Grigas [16] devised the “unambiguous” regret (also called unambiguous SPO Loss): $l_{\text{URegret}}(\hat{c}, c) = \max_{w \in W^*(c)} c^T w - z^*(c)$. This loss considers the worst case among all optimal solutions w.r.t. the predicted cost vector. PyEPO provides an evaluation module (Section 4.5) that includes both the regret and the unambiguous regret. However, as Figure 3 shows, the
regret and the unambiguous regret are almost the same in all training procedures. Therefore, although unambiguous regret is more theoretically rigorous, it is not necessary to consider it in practice.

Besides regret, decision error can also be defined as the difference between the true solution and its prediction, such as Hamming distance of solutions [35] and squared error of the solutions [6]. In addition, Dalle et al. [10] also considered treating the objective value $c^\top w^*$ itself as a loss.

3.4 Methodologies

3.4.1 Smart Predict-then-Optimize [10]

To make the decision error differentiable, Elmachtoub and Grigas [10] proposed SPO+, a convex upper bound on the regret:

$$l_{SPO^+}(\hat{c}, c) = -\min_{w \in S} \{(2\hat{c} - c)^\top w\} + 2\hat{c}^\top w^*(c) - z^*(c).$$  \hspace{1cm} (5)

One proposed subgradient for this loss writes as follows:

$$2(w^*(c) - w^*(2\hat{c} - c)) \in \frac{\partial l_{SPO^+}(\hat{c}, c)}{\partial \hat{c}}$$  \hspace{1cm} (6)

Thus, we can use Algorithm 1 to directly minimize $l_{SPO^+}(\hat{c}, c)$ with gradient descent. This algorithm with SPO+ requires solving $\min_{w \in S} (2\hat{c} - c)^\top w$ for each training iteration.

To accelerate the SPO+ training, Mandi et al. [27] employed relaxations (SPO+ Rel) and warm starting (SPO+ WS) to speed-up the optimization. The idea of SPO+ Rel is to use the continuous relaxation of the integer program during training. This simplification greatly reduces the training time at the expense of model performance. Compared to SPO+, the improvement of SPO+ Rel in training efficiency is not negligible. For example, linear programming can be solved in polynomial time while integer programming is worst-case
exponential. In Section 6, we will further discuss this performance-efficiency tradeoff. For \textit{SPO+ WS}, Mandi et al. \cite{mandi2019} suggested using previous solutions as a starting point for the integer programming solver, which potentially improves the efficiency by narrowing down the search space.

### 3.4.2 Differentiable Black-Box Solver \cite{poganic2021}

\textit{DBB} was developed by Pogančić et al. \cite{poganic2021} to estimate gradients from interpolation, replacing the zero gradients in \( \frac{\partial w^*(c)}{\partial c} \). Thus, Pogančić et al. \cite{poganic2021} add a slight perturbation with hyperparameter \( \lambda \) and then utilize finite differences to obtain a zero-order estimate of the gradient. The substitute of \( w^*(c) \) becomes piecewise affine. Therefore, when computing \( w^*(\hat{c}) \), a useful nonzero gradient is obtained at the cost of faithfulness. The forward pass and backward pass are shown in Algorithm 2 and Algorithm 3. The hyperparameter \( \lambda \geq 0 \) controls the interpolation degree. However, compared to \textit{SPO+}, the approximation function of \textit{DBB} is non-convex, so the convergence to a global optimum is compromised, even when the predictor is convex in its parameters.

**Algorithm 2 DBB Forward Pass**

**Require:** \( \hat{c} \)
1: Solve \( w^*(\hat{c}) \)
2: Save \( \hat{c} \) and \( w^*(\hat{c}) \) for backward pass
3: return \( w^*(\hat{c}) \)

**Algorithm 3 DBB Backward Pass**

**Require:** \( \frac{\partial l(\hat{c}, \cdot)}{\partial w^*(\hat{c})}, \lambda \)
1: Load \( \hat{c} \) and \( w^*(\hat{c}) \) from forward pass
2: \( c' := \hat{c} + \lambda \frac{\partial l(\hat{c}, \cdot)}{\partial w^*(\hat{c})} \)
3: Solve \( w^*(c') \)
4: return \( \frac{\partial w^*(\hat{c})}{\partial \hat{c}} := \frac{1}{\lambda}(w^*(c') - w^*(\hat{c})) \)

Similar to \textit{SPO+}, \textit{DBB} requires solving the optimization problem in each training iteration. Thus, utilizing a relaxation/rounding approach may also work for \textit{DBB}. However, Pogančić et al. \cite{poganic2021} did not consider this option. Given the potential efficiency gains that a continuous relaxation can bring, we also conducted experiments for \textit{DBB Rel} in section 6. The same goes for \textit{DP0} and \textit{PFYL} below.

### 3.4.3 Differentiable Perturbed Optimizer \cite{poganic2021}

\textit{DP0} \cite{poganic2021} uses Monte-Carlo samples to estimate solutions, in which the predicted costs \( \hat{c} \) are perturbed with Gaussian noise \( \xi \sim \mathcal{N}(0, I) \). Based on the \( K \) samples of perturbed costs \( \hat{c} + \sigma \xi \), it returns the estimate of the optimal solution expectation

\[
\mathbb{E}_\xi[w^*(\hat{c} + \sigma \xi)] \approx \frac{1}{K} \sum_{k=1}^{K} w^*(\hat{c} + \sigma \xi_k).
\]

\textit{DP0} outputs the expectation of the optimal solution \( \mathbb{E}_\xi[w^*(\hat{c} + \sigma \xi)] \) under a perturbed cost with random noise \( \hat{c} + \sigma \xi \), rather than the optimal solution...
\( w^*(\hat{c}) \) under a fixed cost \( \hat{c} \), where the expectation can be regarded as a combination of proportions of different feasible solutions. Thus, unlike the piecewise constant function \( w^*(\hat{c}) \), \( E_\xi[w^*(\hat{c}+\sigma \xi)] \) varies the proportions in response to the change of \( \hat{c} \), providing a nonzero gradient of \( \hat{c} \):

\[
\frac{\partial E_\xi[w^*(\hat{c}+\sigma \xi)]}{\partial \hat{c}} \approx \frac{1}{K} \sum_{\kappa} w^*(\hat{c}+\sigma \xi_\kappa) \xi_\kappa.
\]

The forward pass and backward pass are as follows:

**Algorithm 4 DPO Forward Pass**

 Require: \( \hat{c}, K, \sigma \)
  1: for sample \( \kappa \in \{1, \ldots, K\} \) do
  2: Generate Gaussian noise \( \xi_\kappa \)
  3: Solve: \( w_{\xi_\kappa} := w^*(\hat{c}+\sigma \xi_\kappa) \)
  4: Save \( w_{\xi_\kappa} \) and \( \xi_\kappa \) for backward pass
  5: end for
  6: return \( \frac{1}{K} \sum_{\kappa} w_{\xi_\kappa} \)

**Algorithm 5 DPO Backward Pass**

 Require: \( \frac{\partial l}{\partial E_\xi[w^*]} \), \( \frac{\partial l}{\partial \hat{c}} \)
  1: Load \( w_{\xi_\kappa} \) and \( \xi_\kappa \) from forward pass
  2: Compute \( \frac{\partial E_\xi[w^*]}{\partial \hat{c}} := \frac{1}{K} \sum_{\kappa} w_{\xi_\kappa} \xi_\kappa \)
  3: Compute \( \frac{\partial l}{\partial \hat{c}} := \frac{\partial l}{\partial E_\xi[w^*]} \frac{\partial E_\xi[w^*]}{\partial \hat{c}} \)
  4: return \( \frac{\partial l}{\partial \hat{c}} \)

### 3.5 Perturbed Fenchel-Young Loss \[6\]

Instead of an arbitrary loss for \( \text{DPO} \), Berthet et al. \[6\] further construct the Fenchel-Young loss \[7\] to directly compute the decision error \( l_{FY}(\hat{c}, w^*(c)) \) and gradient \( \frac{\partial l_{FY}(\hat{c}, w^*(c))}{\partial \hat{c}} \). Compared to \( \text{DPO} \), \( \text{PFYL} \) avoids the inefficient calculation of the Jacobian matrix \( \nabla^T w^*(\hat{c}) \) and includes a theoretically sound loss function.

The loss of \( \text{PFYL} \) is based on Fenchel duality: The expectation of the perturbed minimizer is defined as \( F(c) = E_\xi\{w^*(c + \sigma \xi)\} \), and the dual of \( F(c) \), denoted by \( \Omega(w^*(c)) \), is utilized to define the Fenchel-Young loss:

\[
l_{FY}(\hat{c}, w^*(c)) = \hat{c}^T w^*(c) - F(\hat{c}) - \Omega(w^*(c)),
\]

then the gradient of the loss is

\[
\frac{\partial l_{FY}(\hat{c}, w^*(c))}{\partial \hat{c}} = w^*(c) - \frac{\partial F(\hat{c})}{\partial \hat{c}} = w^*(c) - E_\xi[\arg\min_{w \in S} \{ (\hat{c} + \sigma \xi)^T w \}].
\]

Similar to \( \text{DPO} \), we can estimate the well-defined gradient as

\[
\frac{\partial l_{FY}(\hat{c}, w^*(c))}{\partial \hat{c}} \approx w^*(c) - \frac{1}{K} \sum_{\kappa} \arg\min_{w \in S} \{ (\hat{c} + \sigma \xi_\kappa)^T w \}
\]
4 Implementation and Modeling

The core module of PyEPO is an “autograd” function which is inherited from PyTorch [32]. Such functions implement a forward pass that yields optimal solutions or decision losses directly and a backward pass to obtain non-zero gradients so that the prediction model can learn from the decision error or its surrogates. Thus, our implementation extends PyTorch, which facilitates the deployment of end-to-end predict-then-optimize tasks using any neural network that can be implemented in PyTorch.

We choose GurobiPy [22] and Pyomo [24] to build optimization models. Both GurobiPy and Pyomo are algebraic modeling languages (AMLs) written in Python. GurobiPy is a Python interface to Gurobi, which combines the expressiveness of a modeling language with the flexibility of a programming language. As an official interface of Gurobi, GurobiPy has a simple algebraic syntax and natively supports all features of Gurobi. Considering that users may not have a Gurobi license, we have additionally designed a Pyomo interface as an alternative. As an open-source optimization modeling language, Pyomo supports a variety of solvers, including Gurobi and GLPK. Both of the above provide a natural way to express mathematical programming models. Users without specialized optimization knowledge can easily build and maintain optimization models through high-level algebraic representations. Besides GurobiPy and Pyomo, PyEPO also allows users to construct optimization models from scratch using any algorithm and solver. As a result, fast and flexible model customization for research and production is possible in PyEPO.

![Fig. 4: Parallel efficiency: Although there is additional overhead in creating a new process, parallel computing of SPo+ and DBB with an appropriate number of processors can reduce the training time effectively.](image)

In addition, PyEPO supports parallel computing. For SPo+, DBB, DP0, and PFYL, the computational cost is a major challenge that cannot be ignored, particularly for integer programs. Both require solving an optimization problem per instance to obtain the gradient.
Figure 4 shows the average running time per epoch for a mini-batch gradient descent algorithm with a batch size of 32 as a function of the number of cores. The decrease in running time per epoch is sublinear in the number of cores. This may be explained by the overhead associated with starting up additional cores, which might dominate computation costs. For example, in Figure 4 for the shortest path, the easily solvable polynomial problem, the running time actually increases when the number of cores exceeds 4, while the more complicated $\mathcal{NP}$-complete problem, TSP, continues to benefit slightly from additional cores. Overall, we believe this feature to be crucial for large-scale predict-then-optimize tasks.

4.1 Optimization Model

The first step in using PyEPO is to create an optimization model that inherits from the optModel class. Since PyEPO tackles predict-then-optimize with unknown cost coefficients, it is first necessary to instantiate an optimization model, optModel, with fixed constraints and variable costs. Such an optimization model would accept different cost vectors and be able to find the corresponding optimal solutions with a fixed set of constraints. The construction of optModel is separated from the autograd functions (see Section 4.2). An instance of optModel will be passed as an argument into the autograd functions.

4.1.1 Optimization Model from Scratch

In PyEPO, the optModel works as a black-box, which means that we do not specifically require a certain algorithm or a certain solver. This design is intended to give users more freedom to customize their tasks. To build an optModel from scratch, users need to override abstract methods _getModel to build a model and get its variables, setObj to set the objective function with a given cost vector, and solve to find an optimal solution. In addition, optModel provides an attribute modelSense to indicate whether the problem is one of minimization or maximization. The following shortest path example uses the Python library NetworkX [23] and its built-in Dijkstra’s algorithm:

```python
import networkx as nx
from pyepo import EPO
from pyepo.model.opt import optModel

class myShortestPathModel(optModel):
    def __init__(self):
        self.modelSense = EPO.MINIMIZE
        self.grid = (5,5) # graph size
        self.arcs = self._getArcs() # list of arcs
        super().__init__()

    def _getModel(self):
```
A method to build model

```python
model = nx.Graph()
model.add_edges_from(self.arcs, cost=0)
var = model.edges
return model, var
```

A method to set objective function

```python
def setObj(self, c):
    for i, e in enumerate(self.arcs):
        self._model.edges[e]["cost"] = c[i]
```

A method to solve model

```python
def solve(self):
    s = 0 # source node
    t = self.grid[0] * self.grid[1] - 1 # target node
    path = nx.shortest_path(self._model, weight="cost", source=s, target=t)
    edges = []
    u = 0
    for v in path[1:]:
        edges.append((u,v))
        u = v
    sol = [0] * self.num_cost
    obj = 0
    for i, e in enumerate(self.arcs):
        if e in edges:
            sol[i] = 1
            obj += self._model.edges[e]["cost"]
    return sol, obj
```

A helper method to get list of arcs for grid network

```python
def _getArcs(self):
    arcs = []
    h, w = self.grid
    for i in range(h):
        for j in range(w - 1):
            v = i * w + j
            arcs.append((v, v + 1))
```
for j in range(w):
    v = i * w + j
    arcs.append((v, v + w))
return arcs

4.1.2 Optimization Model with Gurobi

On the other hand, we provide optGrbModel to create an optimization model with GurobiPy. Unlike optModel, optGrbModel is more lightweight but less flexible for users. Let us use the following optimization model (7) as an example, where $c_i$ is an unknown cost coefficient:

$$\max \sum_{i=0}^{4} c_i x_i$$

s.t.  
\begin{align*}
3x_0 + 4x_1 + 3x_2 + 6x_3 + 4x_4 & \leq 12 \\
4x_0 + 5x_1 + 2x_2 + 3x_3 + 5x_4 & \leq 10 \\
5x_0 + 4x_1 + 6x_2 + 2x_3 + 3x_4 & \leq 15 \\
\forall x_i \in \{0, 1\}
\end{align*}

Inheriting optGrbModel is the convenient way to use Gurobi with PyEPO. The only implementation required is to override _getModel and return a Gurobi model and the corresponding decision variables. In addition, there is no need to assign a value to the attribute modelSense in optGrbModel manually. An example for Model (7) is as follows:

```python
import gurobipy as gp
from gurobipy import GRB
from pyepo.model.grb import optGrbModel

class myModel(optGrbModel):
    def _getModel(self):
        m = gp.Model()
        # variables
        x = m.addVars(5, name="x", vtype=GRB.BINARY)
        # sense (must be minimize)
        m.modelSense = GRB.MAXIMIZE
        # constraints
        m.addConstr(3*x[0]+4*x[1]+3*x[2]+6*x[3]+4*x[4]<=12)
        m.addConstr(4*x[0]+5*x[1]+2*x[2]+3*x[3]+5*x[4]<=10)
        m.addConstr(5*x[0]+4*x[1]+6*x[2]+2*x[3]+3*x[4]<=15)
        return m, x

optmodel = myModel()
```
4.1.3 Optimization Model with Pyomo

Similarly, optOmoModel allows modeling mathematical programs with Pyomo. In contrast to optGrbModel, optOmoModel requires an explicit object attribute modelSense. Since Pyomo supports multiple solvers, instantiating an optOmoModel requires a parameter solver to specify the solver. The following is an implementation of problem 7:

```python
from pyomo import environ as pe
from pyepo import EPO
from pyepo.model.omo import optOmoModel

class myModel(optOmoModel):
    def _getModel(self):
        # sense
        self.modelSense = EPO.MAXIMIZE
        # create a model
        m = pe.ConcreteModel()
        # variables
        x = pe.Var([0,1,2,3,4], domain=pe.Binary)
        m.x = x
        # constraints
        m.cons = pe.ConstraintList()
        m.cons.add(3*x[0]+4*x[1]+3*x[2]+6*x[3]+4*x[4] <=12)
        m.cons.add(4*x[0]+5*x[1]+2*x[2]+3*x[3]+5*x[4] <=10)
        m.cons.add(5*x[0]+4*x[1]+6*x[2]+2*x[3]+3*x[4] <=15)
        return m, x

optmodel = myModel(solver="glpk")
```

4.2 Autograd Functions

Training neural networks with modern deep learning libraries such as TensorFlow [1] or PyTorch [33] requires gradient calculations for backpropagation. For this purpose, the numerical technique of automatic differentiation [32] is used. For example, PyTorch provides autograd functions, so that users are allowed to utilize or create functions that automatically compute partial derivatives.

Autograd functions are the core modules of PyEPO that solve and backpropagate the optimization problems with predicted costs. These functions can be integrated with different neural network architectures to achieve end-to-end predict-then-optimize for various tasks. In PyEPO, autograd functions include SPOPlus [16], blackboxOpt [35], perturbedOpt [6], and perturbedFenchelYoung [6].

4.2.1 Function SPOPlus

The function SPOPlus directly calculates SPO+ loss, which measures the decision error of an optimization solve with predicted cost coefficients. This optimization is represented as an instance of optModel and passed into the
SPOPlus as an argument. As shown below, SPOPlus also requires `processes` to specify the number of processes.

```python
from pyepo.func import SPOPlus
# init SPO+ Pytorch function
spop = SPOPlus(optmodel, processes=8)
```

The parameters for the forward pass of SPOPlus are as follows:

- `pred_cost`: a batch of predicted cost vectors, one vector per instance;
- `true_cost`: a batch of true cost vectors, one vector per instance;
- `true_sol`: a batch of true optimal solutions, one vector per instance;
- `true_obj`: a batch of true optimal objective values, one value per instance.

The following code block is the SPOPlus forward pass:

```python
# calculate SPO+ loss
loss = spop(pred_cost, true_cost, true_sol, true_obj)
```

### 4.2.2 Function `blackboxOpt`

SPOPlus directly obtains a loss while `blackboxOpt` provides a solution. Thus, `blackboxOpt` makes it possible to use various loss functions. Compared to SPOPlus, `blackboxOpt` requires an additional parameter `lambd`, which is the interpolation hyperparameter $\lambda$ for the differentiable black-box solver. According to Poganjic et al. [35], the values of $\lambda$ should be between 10 and 20.

```python
from pyepo.func import blackboxOpt
# init DBB solver
dbb = blackboxOpt(optmodel, lambd=10, processes=8)
```

Since `blackboxOpt` works as a differentiable optimizer, there is only one parameter `pred_cost` for the forward pass. As in the code below, the output is the optimal solution for the given predicted cost:

```python
# find optimal solution
pred_sol = dbb(pred_cost)
```

### 4.2.3 Function `perturbedOpt`

Same as `blackboxOpt`, `perturbedOpt` is a differentiable optimizer and provides an “expected solution” for an arbitrary loss function. The hyperparameters for `perturbedOpt` include `n_sample` and `sigma` as the number of Monte-Carlo sample $K$ and the amplitude parameter of the perturbation $\sigma$, respectively.

```python
import pyepo
# init DPO solver
dpo = pyepo.func.perturbedOpt(optmodel, n_samples=3, sigma=1.0, processes=8)
```

Given predicted cost $\hat{c}$, `perturbedOpt` outputs an expected solution by averaging the solutions of `n_sample` randomly perturbed optimization problems:

```python
# find the expected optimal solution
exp_sol = dpo(pred_cost)
```
4.2.4 Function `perturbedFenchelYoung`

`perturbedFenchelYoung` uses a cost prediction $\hat{c}$ and a true solution $w^*(c)$ to compute the Perturbed Fenchel-Young loss $l_{FY}(\hat{c}, w^*(c))$; it requires the same hyperparameters as `perturbedOpt`.

```python
import pyepo

# init Fenchel-Young loss
pfyl = pyepo.func.perturbedFenchelYoung(optmodel, n_samples=3, sigma=1.0, processes=8)
```

The below code block illustrates the calculation of Fenchel-Young loss:

```python
# calculate Fenchel-Young loss
loss = pfyl(pred_cost, true_sol)
```

4.3 The `optDataset` Class for Managing Data

The utilization of decision losses, such as SPO+ and PFYL, necessitates the availability of true optimal solutions. Therefore, to facilitate convenience in PyEPO training and testing, an auxiliary `optDataset` has been introduced, which is not strictly indispensable. `optDataset` stores the features and their associated costs of the objective function and solves optimization problems to get optimal solutions and corresponding objective values.

`optDataset` is extended from PyTorch Dataset. In order to obtain optimal solutions, `optDataset` requires the corresponding `optModel` (see in Section 4.1). The parameters for the `optDataset` are as follows:

- `model`: an instance of `optModel`;
- `feats`: data features;
- `costs`: corresponding costs of objective function;

Then, as the following example, PyTorch DataLoader receives an `optDataset` and wraps the data samples and acts as a sampler that provides an iterable over the given dataset. It is required to provide the batch size which is the number of training samples that will be used in each update of the model parameters.

```python
import pyepo
from torch.utils.data import DataLoader

# build dataset
dataset = pyepo.data.dataset.optDataset(optmodel, feats, costs)

# get data loader
dataloader = DataLoader(dataset, batch_size=32, shuffle=True)
```

By iterating over the DataLoader, we can obtain a batch of features, true costs, optimal solutions, and corresponding objective values:
for x, c, w, z in dataloader:
    # a batch of features
    print(x)
    # a batch of true costs
    print(c)
    # a batch of true optimal solutions
    print(w)
    # a batch of true optimal objective values
    print(z)

4.4 End-to-End Training

The core capability of PyEPO is to build an optimization model, and then embed the optimization model into a PyTorch neural network for the end-to-end training. Here, we build a simple linear regression model in PyTorch as an example:

from torch import nn

# construct linear model
class LinearRegression(nn.Module):
    def __init__(self):
        super(LinearRegression, self).__init__()
        # size of input and output is the size of feature and cost
        self.linear = nn.Linear(num_feat, len_cost)
    def forward(self, x):
        out = self.linear(x)
        return out

# init model
predmodel = LinearRegression()

Then, we can train the prediction model with SPO+ loss to predict unknown cost coefficients, make decisions, and compute decision errors. The training of the prediction model is performed using a stochastic gradient descent (SGD) optimizer. By utilizing PyTorch automatic differentiation capabilities, the gradients of the loss with respect to the model parameters are computed and used to update the model parameters during training.

import torch

# set SGD optimizer
optimizer = torch.optim.SGD(predmodel.parameters(), lr=1e-3)

# training
for epoch in range(num_epochs):
    # iterate features, costs, solutions, and objective values
    for x, c, w, z in dataloader:
        # forward pass
        cp = predmodel(x)  # predict costs
        loss = sopo(cp, c, w, z).mean()  # calculate SPO+ loss
        # backward pass
        optimizer.zero_grad()  # reset gradients to 0
        loss.backward()  # compute gradients
        optimizer.step()  # update model parameters
4.5 Metrics

*PyEPO* provides evaluation functions to measure model performance, in particular the two metrics mentioned in Section 3.3.1 regret and unambiguous regret. We further define the normalized (unambiguous) regret by

$$
\frac{\sum_{i=1}^{n_{test}} l_{\text{Regret}}(\hat{c}_i, c_i)}{\sum_{i=1}^{n_{test}} |z^*(c_i)|}.
$$

Both of them require the following parameters:

- **predmodel**: a regression neural network for cost prediction.
- **optModel**: a *PyEPO* optimization model.
- **dataloader**: a *PyEPO* data loader.

Assume that we have trained a prediction model **predmodel** for an optimization problem **optModel**. To evaluate **predmodel**’s performance on a dataset **dataloader** of **optModel** instances, the following suffices:

```python
from pyepo.metric import regret, unambRegret

# compute normalized regret
regret = regret(predmodel, optmodel, dataloader)

# compute normalized unambiguous regret
uregret = unambRegret(predmodel, optmodel, dataloader)
```

## 5 Benchmark Datasets

### 5.1 Benchmark Datasets from *PyEPO*

In this section, we describe our new datasets designed for the task of end-to-end predict-then-optimize. Overall, we generate datasets in a similar way to Elmachtoub and Grigas [16]. The synthetic dataset $D$ includes features $x$ and cost coefficients $c$: $D = \{(x_1,c_1),(x_2,c_2),..., (x_n,c_n)\}$. The feature vector $x_i \in \mathbb{R}^p$ follows a standard multivariate Gaussian distribution $\mathcal{N}(0,I_p)$ and the corresponding cost vector $c_i \in \mathbb{R}^d$ comes from a (possibly nonlinear) polynomial function of $x_i$ with additional random noise. $\epsilon_{ij} \sim U(1-\bar{\epsilon},1+\bar{\epsilon})$ is the multiplicative noise term for $c_{ij}$, the $j^{th}$ element of cost $c_i$.

Our dataset includes three of the most classical optimization problems: the shortest path problem, the multi-dimensional knapsack problem, and the traveling salesperson problem. *PyEPO* provides functions to generate these data with adjustable data size $n$, number of features $p$, cost vector dimension $d$, polynomial degree $deg$, and noise half-width $\bar{\epsilon}$.

#### 5.1.1 Shortest Path

Following Elmachtoub and Grigas [16], we consider a $h \times w$ grid network and the goal is to find the shortest path [31] from northwest to southeast. We generate a random matrix $B \in \mathbb{R}^{d \times p}$, where $B_{ij}$ follows Bernoulli distribution
with probability 0.5. Then, the cost vector $c_i$ is almost the same as in [10], and is generated from

$$
\left[ \frac{1}{3.5^\text{deg}} \left( \frac{1}{\sqrt{p}} (Bx_i)_j + 3 \right)^\text{deg} + 1 \right] \cdot \epsilon_{ij}.
$$

(8)

The following code generates data for the shortest path on the grid network:

```python
from pyepo.data.shortestpath import genData
x, c = genData(n, p, grid=(h,w), deg=deg, noise_width=e)
```

5.1.2 Multi-Dimensional Knapsack

The multi-dimensional knapsack problem [28] is one of the most well-known integer programming models. It maximizes the value of selected items under multiple resource constraints. Due to its computational complexity, solving this problem can be challenging, especially with the increase in the number of constraints (or resources or knapsacks).

Because we assume that the uncertain coefficients exist only in the objective function, the weights of items are fixed throughout the data. We use $k$ to denote the number of resources; the number of items is the same as the dimension of the cost vector $d$. The weights $W \in \mathbb{R}^{k \times m}$ are sampled from 3 to 8 with a precision of 1 decimal place. With the same $B \in \mathbb{R}^{d \times p}$ as in Section 5.1.1, cost $c_{ij}$ is calculated according to Equation (8).

To generate $k$-dimensional knapsack data, a user simply executes the following:

```python
from pyepo.data.knapsack import genData
W, x, c = genData(n, p, num_item=d, dim=dim, deg=deg, noise_width=e)
```

5.1.3 Traveling Salesperson

As one of the most famous combinatorial optimization problems, the traveling salesperson problem (TSP) aims to find the shortest possible tour that visits every node exactly once. Here, we introduce the symmetric TSP with the number of nodes to be visited $v$.

PyEPO generates costs from a distance matrix. The distance is the sum of two parts: one comes from Euclidean distance, and the other is derived from a polynomial function of the features. For Euclidean distance, we create coordinates from the mixture of Gaussian distribution $\mathcal{N}(0, I)$ and uniform distribution $U(-2, 2)$. For the function of the features, the polynomial kernel function is

$$
\left( \frac{1}{\sqrt{p}} (Bx)_j + 3 \right)^\text{deg} \cdot \epsilon_{ij},
$$

where the elements of $B$ come from the multiplication of Bernoulli $B(0.5)$ and uniform $U(-2, 2)$.

An example of a TSP data generation is as follows:

```python
from pyepo.data.tsp import genData
x, c = genData(n, p, num_node=v, deg=deg, noise_width=e)
```
5.2 Warcraft Terrain Map Images

Pogančić et al. [35] proposed a dataset of maps from the popular video game Warcraft (refer to Figure 5), which allows learning the shortest path from RGB terrain images. It is a remarkable benchmark due to its image inputs, a modality that was not explored in other work in this area. In accordance with the experiment of Pogančić et al. [35] and Berthet et al. [6], we utilize 96 × 96 RGB images for the shortest path on 12 × 12 grid networks.

Fig. 5: Warcraft terrain shortest path dataset: (Left) Each input feature is a \( k \times k \) terrain map image as a grid of tiles; (Middle) the respective weights is a matrix indicating traveling costs; (Right) the corresponding binary matrix represents the shortest path from top left to bottom right.

6 Empirical Evaluation for PyEPO Datasets

In this section, we present experimental results for the benchmark datasets of Section 5.1. The experiments aimed to investigate the training time and normalized regret (as defined in Section 4.5) on a test set of size \( n_{\text{test}} = 1000 \).

As Table 3 shows, the methods we compare include the two-stage approach with different predictors and \( \text{SPO}^+ / \text{DBB} / \text{PFYL} \) with a linear prediction model \( g(x; \theta) \). Notably, \( \text{DPO} \) was not shown due to its overall subpar performance.

Unlike direct decision loss functions \( \text{SPO}^+ \) and \( \text{PFYL} \), \( \text{DBB} \) and \( \text{DPO} \) allow the use of arbitrary loss functions, and the flexibility in the loss could be useful for different problems. In the original paper, Pogančić et al. [35] used the Hamming distance between the true optimum and the predicted solution, while Berthet et al. [6] employed the squared difference between solutions. However, in our experiments, compared to the regret, \( \text{DBB} \) using the Hamming distance is only sensible for the shortest path problem but leads to much worse decisions in knapsack and TSP. For the sake of consistency, we only use regret (4) as the loss for \( \text{DBB} \).
Table 3: Methods compared in the experiments.

| Method       | Description                                                                 |
|--------------|------------------------------------------------------------------------------|
| 2-stage LR   | Percentage method where the predictor is a linear regression                |
| 2-stage RF   | Two-stage method where the predictor is a random forest with default parameters |
| 2-stage Auto | Two-stage method where the predictor is Auto-Sklearn[18] with 10 minutes time limit and uses MSE as metric |
| SPO+         | Linear model with SPO+ loss [16]                                            |
| PFYL         | Linear model with perturbed Fenchel-Young loss [6]                          |
| DBB          | Linear model with differentiable black-box optimizer [35]                  |
| SPO+ Rel     | Linear model with SPO+ loss [16], using linear relaxation for training      |
| PFYL Rel     | Linear model with perturbed Fenchel-Young loss [6], using linear relaxation for training |
| DBB Rel      | Linear model with differentiable black-box optimizer [35], using linear relaxation for training |
| SPO+ L1      | Linear model with SPO+ loss [16], using $l_1$ regularization for cost       |
| SPO+ L2      | Linear model with SPO+ loss [16], using $l_2$ regularization for cost       |
| PFYL L1      | Linear model with perturbed Fenchel-Young loss [6], using $l_1$ regularization for cost |
| PFYL L2      | Linear model with perturbed Fenchel-Young loss [6], using $l_2$ regularization for cost |
| DBB L1       | Linear model with differentiable black-box optimizer [35], using $l_1$ regularization for cost |
| DBB L2       | Linear model with differentiable black-box optimizer [35], using $l_2$ regularization for cost |

6.1 Performance Comparison between Different Methods

We compare the performance between two-stage methods, SPO+, PFYL, and DBB with varying training data size $n \in \{100, 1000, 5000\}$, polynomial degree $\text{deg} \in \{1, 2, 4, 6\}$, and noise half-width $\bar{\epsilon} \in \{0.0, 0.5\}$. We then conduct small-scale experiments on the validation set to select gradient descent hyperparameters, namely the batch size, learning rate, and momentum for the shortest path, knapsack, and TSP in SPO+, PFYL, and DBB. The hyperparameter tuning uses a limited random search in the space of hyperparameter configurations. Thus, there is no guarantee of the best performance in the results. For PFYL, we arbitrarily set the number of samples $K = 1$ and the perturbation amplitude $\sigma = 1.0$. We repeated all experiments 10 times, each with a different $x$, $B$, and $\epsilon$ to generate 10 different training/validation/test datasets. We use boxplots to summarize the statistical outcomes.

Table 4: Problem Parameters for Performance Comparison
We generate synthetic datasets with parameters in Table 4 so the dimensions of the cost vectors $d$ are 40, 32, and 190, respectively. For the TSP, we use the Dantzig–Fulkerson–Johnson (DFJ) formulation because it is faster to solve than alternatives.

Fig. 6: Normalized regret for the shortest path problem on the test set: The size of the grid network is $5 \times 5$. The methods in the experiment include two-stage approaches with linear regression, random forest, and Auto-Sklearn and end-to-end learning such as SPO+, PFYL, and DBB. The normalized regret is visualized under different sample sizes, noise half-width, and polynomial degrees. For normalized regret, lower is better.

Figures 6, 7, and 8 summarize the performance comparison for the shortest path problem, 2D knapsack problem, and traveling salesperson problem. These figures should be read as follows: the left column is for noise-free costs (easier), while the right column includes noise. Each row of figures is for a training set size in increasing order. Within each figure and from left to right, the degree of the polynomial that generates the costs from the feature vector increases. Within each such polynomial degree, the different methods’ box-plots are shown, summarizing the test set normalized regret results for the 10 different experiments; lower is better.
Fig. 7: Normalized regret for the 2D knapsack problem on the test set: There are 32 items, and the capacity of the two resources is 20. The methods in the experiment include two-stage approaches with linear regression, random forest and Auto-Sklearn and end-to-end learning such as SP0+, PFYL, and DBB. The normalized regret is visualized under different sample sizes, noise half-width, and polynomial degrees. For normalized regret, lower is better.

Two-stage linear regression (2-stage LR) performs well at lower polynomial degrees but loses its advantage at higher polynomial degrees. The two-stage random forest (2-stage RF) is robust at high polynomial degrees but requires a large amount of training data. With 5000 data samples, random forest achieves the best performance in many cases. The two-stage method with automated hyperparameter tuning using the Auto-Sklearn tool [15] (which will be discussed further in the next section, Section 6.2) is attractive: despite tuning for lower prediction error (not decision error), Auto-Sklearn effectively reduces the regret so that it usually performs better than two-stage linear regression and random forest. However, with the increase of input and output dimension, Auto-Sklearn fails to be competitive for the TSP (shown in Figure 8).

SP0+ and PFYL show their advantage: they perform best, or at least relatively well, in all cases. SP0+ and PFYL are comparable to linear regression under low polynomial degrees and depend less on the sample size than random forest. At high polynomial degrees, SP0+ and PFYL outperform Auto-Sklearn,
which exposes the limitations of the two-stage approach. Compared to the SPO+, the PFYL method provides an additional benefit in that it does not necessitate the presence of true costs \( c \) within the training dataset.

**Finding #1**

SPO+ and PFYL can robustly achieve relatively good decisions under different scenarios, often outperforming two-stage baselines.

6.2 Two-stage Method with Automated Hyperparameter Tuning

This method leverages the sophisticated Auto-Sklearn [15] tool that uses bayesian optimization methods for automated hyperparameter tuning of Scikit-Learn regression models. The metric of “2-stage Auto” is the mean squared error of
the predicted costs, which does not reduce decision error directly. Because of the limitation of multioutput regression in *Auto-Sklearn* v0.14.6, the choices of the predictor in 2-stage Auto only include five models: k-nearest neighbor (KNN), decision tree, random forest, extra-trees, and Gaussian process. Even with these limitations, *Auto-Sklearn* can achieve a low regret. Although the training of 2-stage Auto is time-consuming, it is still a competitive method.

**Finding #2**

Even with successful model selection and hyperparameter tuning, the two-stage method performs worse than *SPO+* in terms of decision quality, which substantiates the value of the end-to-end approach.

6.3 Exact Method and Relaxation

Training *SPO+, PFYL*, and *DBB* with a linear relaxation instead of solving the integer program improves computational efficiency. However, the use of a “weaker” solver theoretically undermines model performance. Therefore, an important question arises about the tradeoff when using a linear relaxation in training. To this end, we compare the performance of end-to-end approaches with their relaxation using 2D knapsack and TSP as examples. We use the same instances, models, and hyperparameters as before.

*Fig. 9: Average training time per iteration for exact and relaxation methods with standard deviation error bars: We visualized the mean training time with standard deviation for the Knapsack and TSP; lower is better.*

There are several integer programming formulations for the TSP. Besides DFJ, we also implemented the Miller-Tucker-Zemlin (MTZ) formulation [30] and the Gavish-Graves (GG) formulation [20]. Although they all have the same integer solution, they differ in their linear relaxations. Since DFJ requires column generation to handle the exponential subtour constraints, its linear relaxation is hard to implement. The GG formulation is shown to have a tighter linear relaxation than MTZ. Thus, we use DFJ for exact *SPO+, PFYL*,
and DBB, and MTZ and GG for the relaxation to investigate the effect of solution quality on regret.

According to Figure 9, using a linear relaxation significantly reduces the running time. As shown in Figure 10, the impact on the performance on knapsack is almost negligible. Interestingly, relaxed methods have the potential to perform better on small data, perhaps because the linear relaxation acts as a regularization to avoid overfitting. For TSP, Figure 10 demonstrates that a tighter bound does reduce the regret, and DBB Rel shows advantages over DBB. Overall, using relaxations achieves fairly good performance with improved computational efficiency. Moreover, formulations with tighter linear relaxation lead to better performance.

Finding #3

End-to-end predict-then-optimize with relaxation has excellent potential to improve computation efficiency at a slight degradation in performance, particularly when the true cost-generating function is not very non-linear.
6.4 Prediction Regularization

As proposed in Elmachtoub and Grigas [10], the mean absolute error \( l_{\text{MAE}}(\hat{c}, c) = \frac{1}{n} \sum \| \hat{c}_i - c_i \|_1 \) or mean squared error \( l_{\text{MSE}}(\hat{c}, c) = \frac{1}{n} \sum \| \hat{c}_i - c_i \|_2^2 \) of the predicted cost vector w.r.t. true cost vector can be added to the decision loss as \( l_1 \) or \( l_2 \) regularizers. When using regularization, we set either the \( l_1 \) regularization parameter \( \phi_1 \) and the \( l_2 \) regularization parameter \( \phi_2 \) from 0.001 to 10 logarithmically. For the experiments, we still use the same instances, model, and hyperparameters as before, while the number of training samples \( n \), the noise half-width \( \bar{\epsilon} \) and, the polynomial degree \( \text{deg} \) are fixed at 1000, 0.5 and 4.

![Graphs showing normalized regret and MSE on the test set](image)

Fig. 11: Normalized regret and MSE on the test set: In these experiments, we compare the performance on SPO+, PFYL, and DBB with different levels of \( l_1 \) or \( l_2 \) regularization and show the trend line with increasing regularization, while 2-Stage LR (green line) is served as the baseline. The normalized regret and MSE under different problems are shown; lower is better.

Based on Fig [11], regularization appears to be a viable strategy for effectively reducing MSE. With the increase of the regularization parameter, all end-to-end methods achieve an MSE which is close to that of the two-stage linear regression approach. In terms of regret, the impact on SPO+ and PFYL is insignificant, while more regularization for DBB has the potential to yield improvements.

Finding #4

\( l_1 \) and \( l_2 \) regularization are deemed to be appealing techniques for enhancing prediction accuracy while simultaneously preserving decision quality.
6.5 Trade-offs between MSE and Regret

Figure 12 examines the prediction-decision trade-off on the shortest path with 100 and 1000 training samples, a 0.5 noise half-width, and polynomial degree 4. We calculate the average MSE and regret for 10 repeated random experiments. Apart from this, mean training time is also annotated, and circle sizes are proportional to it. Finally, we remove the circles of DBB because they are at the right top corner and far worse than other methods.

Fig. 12: MSE v.s. Regret: The result covers different two-stage methods, SPO+, PFYL, and their relaxations. DBB is omitted because it is far away from others. The size of the circles is proportional to the training time (Sec), so the smaller is better.

Figure 12 demonstrates that SPO+ and PFYL can reach a low decision error, especially with large training sets, at the cost of higher prediction errors. Moreover, the MSE of PFYL’s predictions is significantly larger than that of SPO+. Further examination reveals that the higher prediction error of SPO+ and PFYL comes mainly from multiplicative shifts in the predicted cost values, which does not alter the optima of an optimization problem with a linear objective function. In addition, training with Auto-Sklearn, which comes from
automated algorithm selection and hyperparameter tuning, is time-consuming
but provides both high-quality prediction error and decision error. However,
compared to $\text{SPO}^+$ and $\text{PFYL}$, even the competitive 2-stage Auto model does
not have an advantage in decision-making with 1000 training data samples.

Inspired by Sec 6.4, we further add $l_2$ regularization with parameter $\phi_2 = 1.0$ for $\text{SPO}^+$ and $\text{PFYL}$, and refer to these as $\text{SPO}^+ L2$ and $\text{PFYL} L2$. Fig
13 shows that the correct amount of prediction regularization can achieve a
favorable balance between MSE and regret, sometimes even reducing the regret
compared to the unregularized variants.

Finding #5

Generally, $\text{SPO}^+$ and $\text{PFYL}$ can achieve good decisions at the cost of pre-
diction accuracy. If one is seeking a balanced tradeoff between decision
quality and prediction accuracy, an end-to-end method with prediction
regularization may be preferable.

7 Empirical Evaluation for Image-Based Shortest Path

Following Pogančić et al. [35] and Berthet et al. [6], we employ a truncated
ResNet18 convolutional neural network (CNN) architecture consisting of the
first five layers on Warcraft terrain images (refer to Section 5.2). As Table 5
shows, the methods we compare include a two-stage method, $\text{SPO}^+$, $\text{DBB}$,
and PFYL with truncated ResNet18. We train the CNN over 50 epochs with batches of size 70. The learning rate is set to 0.0005 decaying at the epochs 30 and 40, and the hyperparameters $n = 1$, $\sigma = 1$ for DP0 and PFYL, $\lambda = 10$ for DBB. We use the Hamming distance for DBB and the squared error of solutions for DP0, which are the loss functions used in the original papers.

| Method | Description |
|--------|-------------|
| 2S     | Two-stage method where the predictor is a truncated ResNet18 |
| SPO+   | Truncated ResNet18 with SPO+ loss [16] |
| DBB    | Truncated ResNet18 with differentiable black-box optimizer and Hamming distance loss [35] |
| DPO    | Truncated ResNet18 with differentiable perturbed optimizer and squared error loss [6] |
| PFYL   | Truncated ResNet18 with perturbed Fenchel-Young loss [6] |

Table 5: Methods compared in the experiments.

The sample size of the test set $n_{test}$ is 1000. To evaluate our methods, we compute the relative regret $\frac{c^T w^*(c) - z^*(c)}{z^*(c)}$ and path accuracy $\sum_{d=1}^{d} 1(z^*(c)_j = z^*(\hat{c})_j)$ per instance on the test set; the latter is simply the fraction of edges in the “predicted” solution that are also in the optimal solution.

As shown in Figure 14, the two-stage method, SPO+ and PFYL, achieve comparable levels of performance in predicting the shortest path on the Warcraft terrain, while PFYL obtains solutions that agree the most with the optima (i.e., highest Path Accuracy). It seems that the Warcraft shortest path problem may not require end-to-end learning. However, it is noteworthy that PFYL, despite lacking knowledge of the true costs, yields a competitive result, encouraging researchers to broaden the applications for end-to-end learning.

Fig. 14: Learning curve, relative regret, and path accuracy for the shortest path problem on the test set: The methods in the experiment include a two-stage neural network, SPO+, DBB, DP0, and PFYL. The learning curve shows relative regret on the test set, and the box plot demonstrates the distribution of relative regret on the test set. For relative regret, lower is better.
Finding #6

End-to-end learning is effective in rich contextual features such as images. Moreover, the study highlights that PFYL can achieve impressive performance levels, even without knowing the costs during training.

8 Conclusion

Because of the lack of easy-to-use generic tools, the potential power of the end-to-end predict-then-optimize has been underestimated or even overlooked in various applications. Our PyEPO package aims to alleviate barriers between the theory and practice of the end-to-end approach.

PyEPO, the PyTorch-based end-to-end predict-then-optimize tool, is specifically designed for linear objective functions, including linear programming and (mixed) integer programming. The tool is extended from the automatic differentiation function of PyTorch, one of the most widespread open-source machine learning frameworks. Hence, PyEPO allows leveraging numerous state-of-art deep learning models and techniques as implemented in PyTorch.

PyEPO allows users to build optimization problems as black boxes or by leveraging interfaces to GurobiPy and Pyomo, thus providing broad compatibility with high-level modeling languages and both commercial and open-source solvers.

With the PyEPO framework, we generate three synthetic datasets and incorporate one image dataset from the literature. Comprehensive experiments and analyses are conducted with these datasets. The results show that the end-to-end methods achieved excellent improvement in decision quality over two-stage methods in many cases. In addition, the end-to-end models can benefit from using relaxations and regularization. The code repository includes step-by-step tutorials that allow new users to replicate the experiments presented in this paper or use them as a starting point for their own applications. The future development efforts of PyEPO include:

- New applications and new optimization problems, including linear objective functions with mixed-integer variables or non-linear constraints;
- Additional variations and improvements to current approaches such as warm starting and training speed up;
- Novel training methods that leverage the gradient computation features that PyEPO provides;
- Other existing end-to-end predict-then-optimize approaches, such as QPTL and its variants.
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9 Statements and Declarations

9.1 Funding

This work was supported by funding from a SCALE AI Research Chair and an NSERC Discovery Grant.

9.2 Author Contributions

Tang and Khalil contributed to the conception and design of the project. Software development, data generation, software testing, and benchmarking experiments were performed by Tang. Tang wrote the first draft of the submission. Tang and Khalil contributed to finalizing the submission. Both authors read and approved the final manuscript.

9.3 Competing Interests

The authors have no relevant financial or non-financial interests to disclose.