Contrastive Predict-and-Search for Mixed Integer Linear Programs

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Abstract

Mixed integer linear programs (MILP) are flexible and powerful tools for modeling and solving many difficult real-world combinatorial optimization problems. In this paper, we propose a novel machine learning (ML)-based framework *ConPaS* that learns to predict solutions to MILPs with contrastive learning. For training, we collect high-quality solutions as positive samples. We also collect low-quality or infeasible solutions as negative samples using novel optimization-based or sampling approaches. We then learn to make discriminative predictions by contrasting the positive and negative samples. During testing, we predict and fix the assignments for a subset of integer variables and then solve the resulting reduced MILP to find high-quality solutions. Empirically, ConPaS achieves state-of-the-art results compared to other ML-based approaches in terms of the quality of and the speed at which solutions are found.

1. Introduction

Combinatorial optimization (CO) concerns a wide variety of real-world problems, including resource allocation (Manne, 1960), traffic management (Luathep et al., 2011), network design (Huang & Dilkina, 2020) and production planning (Pochet & Wolsey, 2006) problems, and the majority of them are NP-hard. Therefore, designing efficient and effective CO algorithms is important and challenging. Mixed integer linear programs (MILP) can flexibly encode and solve a broad family of CO. A MILP is a mathematical program that optimizes a linear objective subject to linear constraints, with some of the variables constrained to take integer values. Significant research and engineering effort has been dedicated to developing MILP solvers, such as SCIP (Maher et al., 2017), Gurobi (Gurobi Optimization, LLC, 2022) and CPLEX (Cplex, 2009). The backbones of these solvers are Branch-and-Bound (BnB) (Land & Doig, 2010), Branch-and-Cut (Mitchell, 2002) or Branch-Cut-and-Price (Desrosiers & Lübbecke, 2011), which are optimal tree search algorithms enhanced by a group of heuristics.

MILPs from the same application domain often share similar structures and characteristics in many real-world settings. The performance of MILP solvers crucially depends on how effective the heuristics are for that application. Recently, there has been an increased interest in data-driven heuristic designs for MILP for various decision-making in BnB (see Section 3.2 for a summary). Another line of research focuses on heuristics that generate high-quality solutions for MILPs. In particular, it focuses on generating partial assignments of high-quality feasible solutions. Previously, Nair et al. (2020) propose Neural Diving (ND), where they learn to partially assign values to integer variables and delegate the reduced sub-MILP to a MILP solver, e.g., SCIP. The fraction of variables to assign values to is controlled by a hyperparameter called the coverage rate. A SelectiveNet (Geifman & El-Yaniv, 2019) is trained for each coverage rate that jointly decides which variables to fix and the values to fix to during testing. The main two disadvantages of ND are that (1) enforcing variables to fixed values leads to low-quality or infeasible solutions if the predictions are not accurate enough and (2) it requires training multiple SelectiveNet to obtain the appropriate coverage rate, which is computationally expensive. To mitigate these issues, Han et al. (2022) propose a Predict-and-Search (PaS) framework that deploys a search inspired by the trust region method. Instead of fixing variables, PaS searches for high-quality solutions within a pre-defined proximity of the predicted partial assignment, which allows better feasibility and finding higher-quality solutions than ND. For both ND and PaS, the effectiveness (i.e., the quality of the solution found) and efficiency (i.e., the speed at which high-quality solutions are found) depend on the accuracy of the machine learning (ML) prediction and the number of variables (controlled by hyperparameters) whose values to fix.

In this paper, we propose a novel ML-based framework *ConPaS*, **Con**trastive **P**redict-**a**nd-**S**earch for MILPs. Inspired by the recent success in contrastive learning (CL) for refining solutions with large neighborhood search (LNS)

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for MILPs (Huang et al., 2023), ConPaS leverages CL for another important task of learning to construct high-quality (partial) solutions to MILPs. A key to adapting CL to this task is devising an appropriate and effective way of collecting positive and negative samples in this new context. Similar to both ND (Nair et al., 2020) and PaS (Han et al., 2022), we collect a set of optimal and near-optimal solutions as *positive samples*; but different from ND and PaS, we additionally collect *negative samples* for CL. We propose to collect two types of negative samples - infeasible solutions and low-quality solutions that are similar to the positive samples - with novel approaches tailored to our task. For infeasible solutions, we use a sampling approach that randomly perturbs a small fraction of the positive samples. For low-quality solutions, we formulate the task as a maximin optimization. During training, instead of using a binary cross entropy loss to penalize the inaccurate predictions for each variable separately, we use a contrastive loss that encourages the model to predict solutions that are similar to the positive samples but dissimilar to the negative ones, with similarity measured by dot products (Oord et al., 2018; He et al., 2020).

Empirically, we test ConPaS on a variety of MILP benchmarks, including problems from the NeurIPS Machine Learning for Combinatorial Optimization (ML4CO) competition (Gasse et al., 2022). We show that ConPaS achieves state-of-the-art anytime performance on finding high-quality solutions to MILPs, significantly outperforming other learning-based methods such as ND and PaS in terms of solution quality and speed. In addition, ConPaS shows great generalization performance on test instances that are 50% larger than the training instances.

2. Background

We first define mixed integer linear programs and then provide detailed introductions to both Neural Diving (Nair et al., 2020) and Predict-and-Search (Han et al., 2022).

2.1. Mixed Integer Linear Programming

A *mixed integer linear program (MILP)* $M = (\boldsymbol{A}, \boldsymbol{b}, \boldsymbol{c}, q)$ is defined as

$$\min \boldsymbol{c}^\mathsf{T}\boldsymbol{x} \quad \text{s.t. } \boldsymbol{A}\boldsymbol{x} \leq \boldsymbol{b} \text{ and } \boldsymbol{x} \in \{0,1\}^q \times \mathbb{R}^{n-q}, \quad (1)$$

where $\boldsymbol{x} = (x_1, \ldots, x_n)^\mathsf{T}$ denotes the q binary variables and $n-q$ continuous variables to be optimized, $\boldsymbol{c} \in \mathbb{R}^n$ is the vector of objective coefficients, $\boldsymbol{A} \in \mathbb{R}^{m \times n}$ and $\boldsymbol{b} \in \mathbb{R}^m$ specify m linear constraints. A solution $\boldsymbol{x}$ is *feasible* if it satisfies all the constraints. This paper focuses on the mixed-binary formulation above; however, our approach can also handle general integers using the same engineering techniques introduced in (Nair et al., 2020).

2.2. Neural Diving

Neural Diving (ND) (Nair et al., 2020) learns to generate a Bernoulli distribution for the solution values of binary variables. It learns the conditional distribution of the solution $\boldsymbol{x}$ given a MILP $M = (\boldsymbol{A}, \boldsymbol{b}, \boldsymbol{c}, q)$ defined as

$$p(\boldsymbol{x}|M) = \frac{\exp(-E(\boldsymbol{x}|M))}{\sum_{\boldsymbol{x}' \in \mathcal{S}_\mathsf{p}^M} \exp(-E(\boldsymbol{x}'|M))},$$

where $\mathcal{S}_\mathsf{p}^M$ is a set of optimal or near-optimal solutions to M and $E(\boldsymbol{x}|M)$ is an energy function of a solution $\boldsymbol{x}$ defined as $\boldsymbol{c}^\mathsf{T}\boldsymbol{x}$ if $\boldsymbol{x}$ is feasible or ∞ otherwise. ND learns $\boldsymbol{p_\theta}(\boldsymbol{x}|M)$ parameterized by a graph convolutional network to approximate $p(\boldsymbol{x}|M)$ assuming conditional independence between variables $p(\boldsymbol{x}|M) \approx \prod_{i \leq q} p_\theta(x_i|M)$. Since the full prediction $\boldsymbol{p}_\theta(\boldsymbol{x}|M)$ might not give a feasible solution, ND predicts only a partial solution controlled by the coverage rates and employs SelectiveNet (Geifman & El-Yaniv, 2019) to learn which variables' values to predict for each coverage rates. ND uses binary cross-entropy loss combined with the loss function for SelectiveNet to train the neural network. During testing, the input MILP M is then reduced to solving a smaller MILP after fixing the selected variables.

2.3. Predict-and-Search

Predict-and-Search (PaS) (Han et al., 2022) uses the same framework as ND to learn to predict $p(\boldsymbol{x}|M)$. Instead of using SelectiveNet to learn to fix variables, PaS searches for near-optimal solutions within a neighborhood based on the prediction. Specifically, given the prediction $p_\theta(x_i|M)$ for each binary variable, PaS greedily selects k_0 binary variables $\mathcal{X}_0$ with the smallest $p_\theta(x_i|M)$ and k_1 binary variables $\mathcal{X}_1$ with the largest $p_\theta(x_i|M)$, such that $\mathcal{X}_0$ and $\mathcal{X}_1$ are disjoint ($k_0 + k_1 \leq q$). PaS fixes all variables in $\mathcal{X}_0$ to 0 and $\mathcal{X}_1$ to 1 in the sub-MILP but also allows $\Delta \geq 0$ of the fixed variables to be flipped when solving it. Formally, let

$$B(\mathcal{X}_0, \mathcal{X}_1, \Delta) = \{\boldsymbol{x} : \sum_{x_i \in \mathcal{X}_0} x_i + \sum_{x_i \in \mathcal{X}_1} 1 - x_i \leq \Delta\}$$

and D be the feasible region of the original MILP, PaS solves the following optimization problem:

$$\min \boldsymbol{c}^\mathsf{T}\boldsymbol{x} \quad \text{s.t. } \boldsymbol{x} \in D \cap B(\mathcal{X}_0, \mathcal{X}_1, \Delta). \quad (2)$$

Restricting the solution space to $B(\mathcal{X}_0, \mathcal{X}_1, \Delta)$ can be seen as a generalization of the fixing strategy employed in ND where $\Delta = 0$. Though in ND, $\mathcal{X}_0$ and $\mathcal{X}_1$ are constructed using sampling methods based on the neural network output.

3. Related Work

In this section, we first summarize other related works on solution predictions for CO. We then summarize related works on MILP solving using machine learning and existing CL methods for solving CO problems.

3.1. Solution Predictions for CO

There are other works on learning to predict solutions to MILPs in addition to ND and PaS. Ding et al. (2020) learn to predict backbone variables (Dubois & Dequen, 2001) whose values stay unchanged across different optimal and near-optimal solutions and then search for optimal solutions based on the predicted backbone variables. However, this approach does not apply to many CO problems since backbone variables do not necessarily exist. Recently, Yoon et al. (2023) propose threshold-aware learning to optimize the coverage rate in ND and is one of the state-of-the-art approaches[1]. However, this approach also fixes variables when solving the sub-MILP. Khalil et al. (2022) and Li et al. (2018) learn to guide decision-making, such as warm-starting and node selection, in CO solvers, such as MIP solvers and local search, via solution predictions.

3.2. Machine Learning-Guided MILP solving

Several studies have applied ML to improve BnB for MILP solving. A huge body of such studies focuses on learning to either select variables to branch on (Khalil et al., 2016; Gasse et al., 2019; Gupta et al., 2020; Zarpellon et al., 2021) or select nodes to expand (He et al., 2014; Labassi et al., 2022). There are also a few studies on learning to schedule and run primal heuristics (Khalil et al., 2017; Chmiela et al., 2021) and to select cutting planes (Tang et al., 2020; Paulus et al., 2022; Huang et al., 2022). Large Neighborhood Search is a popular heuristic search for MILPs to find high-quality primal solutions quickly. Several learning methods (Song et al., 2020; Sonnerat et al., 2021; Wu et al., 2021; Huang et al., 2023) have been proposed to guide selecting partial solutions to iteratively refine in the search.

3.3. Contrastive Learning for CO

Contrastive learning has been studied extensively for visual representations (Hjelm et al., 2019; He et al., 2020; Chen et al., 2020) and graph representations (You et al., 2020; Tong et al., 2021) but it has not been explored much for solving CO problems. Mulamba et al. (2021) derive a contrastive loss for decision-focused learning to solve CO problems with uncertain inputs that can be learned from historical data, where they view non-optimal solutions as negative samples. Duan et al. (2022) pre-train good representations for the boolean satisfiability problem with CL.

In a closely related work, Huang et al. (2023) propose CL-LNS that uses CL to learn heuristics to refine solutions for MILP in LNS. In contrast, ConPaS learns to construct a portion of a high-quality solution from scratch and then search for it. ConPaS uses a novel data collection for negative samples and a novel contrastive loss function that considers positive samples with different qualities. While CL-LNS has a limited application to only LNS, the prediction from ConPaS's ML model can be useful in different search algorithms for MILP. First, ConPaS and CL-LNS are complementary to each other and ConPaS can be used to warm start CL-LNS (or any variants of LNS), similar to what proposed in (Sonnerat et al., 2021). One could also leverage the prediction from ConPaS to assign variable branching priorities or generate cuts to improve the performance of BnB. In addition to CL-LNS, CL has also been applied to predict branching priorities for variables in BnB for MILP solving (Cai et al., 2024).

[1]We do not compare with this approach (Yoon et al., 2023) since it is concurrent with our work and the authors are not ready to share their code when we contacted them.

4. Contrastive Predict-and-Search

In this section, we introduce our novel framework *ConPaS*, **Con**trastive **P**redict-**a**nd-**S**earch for MILPs. For a given MILP M, our goal is to use CL to predict the conditional distribution of the solution $p(\boldsymbol{x}|M)$, such that it leads to high-quality solutions fast when it is used to guide downstream MILP solving. In this paper, we mainly focus on using the prediction in Predict-and-Search (optimization problems (2)) following Han et al. (2022). However, such prediction can be used to decompose the feasible regions of the input MILP for exact solving (Ding et al., 2020) or seed LNS with a better primal solution for heuristic solving (Sonnerat et al., 2021). We employ CL rather than other learning techniques because it has been theoretically demonstrated to be effective (Tian, 2022) and has empirically outperformed alternative approaches in related combinatorial optimization problems (Duan et al., 2022; Huang et al., 2023; Mulamba et al., 2021). Figure 1 gives an overview of ConPaS. Next, we describe our novel data collection, our supervised CL and how we apply solution predictions in the search.

4.1. Training Data Collection

In ConPaS, we use CL to learn to make discriminative predictions of optimal solutions by contrasting positive and negative samples. Since finding good assignments for integer variables is essentially the most challenging part of solving a MILP, we follow previous work (Nair et al., 2020) to learn $p(\boldsymbol{x}|M)$ approximately as $\prod_{i\leq q} p_\theta(x_i|M)$ where we mainly focus on predicting $p_\theta(x_i|M)$ for binary variables ($i \leq q$). Therefore, our definition of positive and negative samples of solutions mainly concerns partial solutions on binary variables (since the optimal solutions for continuous variables can be computed in polynomial time once the binary ones are fixed). Now, we describe how we collect positive and negative samples.

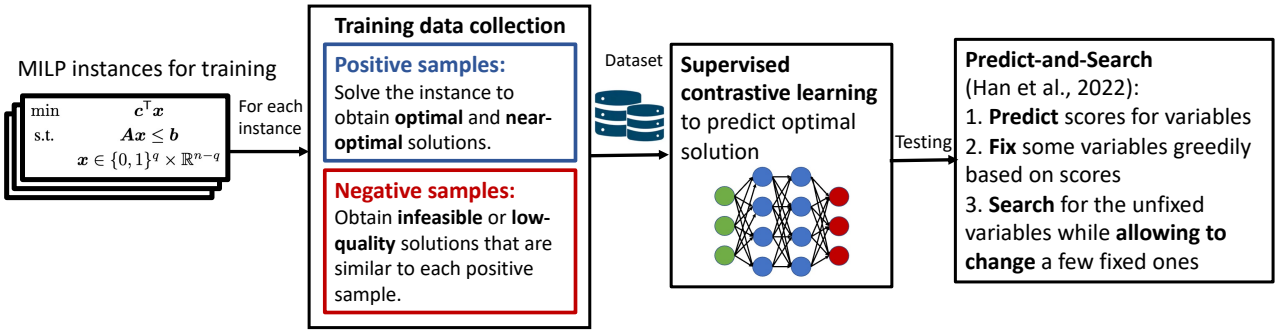


Figure 1: Overview of ConPaS. For training, we collect data from a set of MILP instances, including positive samples that are optimal and near-optimal solutions. We have two variants of ConPaS, namely ConPaS-LQ and ConPaS-Inf, that collect negative samples that are low-quality or infeasible solutions, respectively. We use the data in supervised CL to predict optimal solutions. During testing, the predictions are used in Predict-and-Search (Han et al., 2022).

4.1.1. Positive Samples Collection

For a given MILP M, we collect a set of optimal or near-optimal solutions $\mathcal{S}_{\mathsf{p}}^M$ as our positive samples following previous works (Nair et al., 2020; Han et al., 2022). This is done by solving M exhaustively with a MILP solver and collecting up to u_{p} solutions with the minimum objective values. In experiments, u_{p} is set to 50.

4.1.2. Negative Samples Collection

Negative samples are critical parts of CL to help distinguish between high-quality and low-quality (or even infeasible) solutions. We propose to collect negative samples that are similar to the positive ones. From a theoretical point of view, the InfoNCE loss (Oord et al., 2018; He et al., 2020) we use for training later can automatically focus on hard negative pairs (i.e., samples with similar representation but of very different qualities) and learn representations to separate them apart (Tian, 2022).

Given a MILP M, we collect a set of u_{n} negative samples $\mathcal{S}_{\mathsf{n}}^M$ where $u_{\mathsf{n}} = \beta|\mathcal{S}_{\mathsf{p}}^M|$ and β is a hyperparameter to control the ratio between the number of positive and negative samples. In experiments, β is set to 10. We propose two novel approaches to collect them: (1) a sampling approach to collect infeasible solutions and (2) an optimization-based approach to collect low-quality solutions.

Infeasible Solutions as Negative Samples. We introduce a sampling approach. For each positive sample $\boldsymbol{x} \in \mathcal{S}_{\mathsf{p}}^M$, we collect β infeasible solutions as negative samples. We randomly perturb 10% of the binary variable values in $\boldsymbol{x}$ (i.e., flipping from 0 to 1 or 1 to 0). If the MILP M contains only binary variables, we validate that the perturbed solutions are indeed infeasible if they violate at least one constraint in M. If M contains both binary and continuous variables, we fix the binary variables to the values in the perturbed solutions and ensure that no feasible assignment of the continuous variables exists using a MILP solver. If less than β negative samples are found after validating 2β perturbed samples, we increase the perturbation rate by 5% and repeat the same process until we have β samples.

Low-Quality Solutions as Negative Samples. We introduce an optimization-based approach. For each positive sample $\boldsymbol{x} = (x_1, \ldots, x_n) \in \mathcal{S}_{\mathsf{p}}^M$, we find the worst β feasible solutions that differ from $\boldsymbol{x}$ in at most 10% of the binary variables. If the MILP $M = (\boldsymbol{A}, \boldsymbol{b}, \boldsymbol{c}, q)$ contains only binary variables, we find negative samples $\boldsymbol{x}'$ by solving the following Local Branching (Fischetti & Lodi, 2003) MILP:

$$\begin{aligned} &\max \boldsymbol{c}^\top \boldsymbol{x}' \\ \text{s.t.} \quad &\boldsymbol{A}\boldsymbol{x}' \le \boldsymbol{b},\, \boldsymbol{x}' \in \{0,1\}^q \times \mathbb{R}^{n-q}, \\ &\textstyle\sum_{i \le q: x_i = 0} x_i' + \sum_{i \le q: x_i = 1} (1 - x_i') \le k. \end{aligned} \tag{3}$$

The above MILP is essentially solving the same problem as M, but with a negated objective function that tries to find solution x' as low-quality as possible and a constraint that allows changing at most k of the binary variables. After solving it, we consider only solutions as negative samples if they are worse than a given threshold. k is initially set to $10\% \times q$, but if less than β negative samples are found with the current k, we increase it by 5% and resolve optimization problem (3). We repeat the same process until we have β negative samples.

If M contains continuous variables, the goal is to find partial solutions on binary variables, such that we get as low-quality solutions $\boldsymbol{x}'$ as possible when we fix the binary values and optimize for the rest of the continuous variables. Formally, solving for the partial solutions on binary vari-

ables $x'_1, \ldots, x'_q$ can be written as a maximin optimization:

$$\begin{aligned} &\max_{x'_1,\ldots,x'_q} \min_{x'_{q+1},\ldots,x'_n} \boldsymbol{c}^\mathsf{T}\boldsymbol{x}' \\ \text{s.t.} \quad &\boldsymbol{A}\boldsymbol{x}' \leq \boldsymbol{b},\, \boldsymbol{x}' \in \{0,1\}^q \times \mathbb{R}^{n-q}, \\ &\textstyle\sum_{i\leq q:x_i=0} x'_i + \sum_{i\leq q:x_i=1}(1-x'_i) \leq k. \end{aligned} \tag{4}$$

Solving the above maximin optimization exactly is prohibitively hard and, to the best of our knowledge, there are no general-purpose solvers for it (Beck & Schmidt, 2021, Chapter 7). Therefore, we use a heuristic approach where we iteratively solve the inner minimization problem and add a constraint $\boldsymbol{c}^\mathsf{T}\boldsymbol{x}' > \boldsymbol{c}^\mathsf{T}\boldsymbol{x}^*$ to enforce the next solution found is strictly better than the current best-found solution $\boldsymbol{x}^*$ to the maximin problem. It terminates until no better solution can be found. For faster convergence, we sometimes enforce the next solution found to be at least $\epsilon > 0$ better than $\boldsymbol{x}^*$, i.e., we add $\boldsymbol{c}^\mathsf{T}\boldsymbol{x}' \geq \boldsymbol{c}^\mathsf{T}\boldsymbol{x}^* + \epsilon$, where ϵ is a hyperparameter tuned adaptively in a binary search manner. If we find less than β samples, we adjust k the same way as in the previous case.

4.2. Supervised Contrastive Learning

In this subsection, we introduce the neural network architecture for ConPaS and describe the contrastive loss for training.

4.2.1. Neural Network Architecture

Following previous work (Han et al., 2022), we use a bipartite graph to represent the input MILP M. The bipartite graph has n variables and m constraints on two sides, respectively, with an edge connecting a variable and a constraint if the variable has a non-zero coefficient in the constraint. Following Nair et al. (2020) and Han et al. (2022), we use node and edge features in the bipartite graph proposed by Gasse et al. (2019). We learn $\boldsymbol{p}_{\boldsymbol{\theta}}(\boldsymbol{x}|M)$ represented by a graph convolutional network (GCN) parameterized by learnable weights $\boldsymbol{\theta}$. The GCN takes the bipartite graph representation of M and the features as input. We perform two rounds of message passing through the GCN to obtain an embedding of the variables, which is then passed through a multi-layer perceptron (MLP) followed by a sigmoid activation layer to obtain the final output $p_{\boldsymbol{\theta}}(x_i|M)$. Details of the GCN architecture are included in Appendix.

4.2.2. Training with a Contrastive Loss

Given a set of MILP instances $\mathcal{M}$ for training, let $\mathcal{D} = \{(\mathcal{S}_\mathsf{p}^M, \mathcal{S}_\mathsf{n}^M) : M \in \mathcal{M}\}$ be the set of positive and negative samples for all training instances. A contrastive loss is a function whose value is low when the predicted $\boldsymbol{p}_{\boldsymbol{\theta}}(\boldsymbol{x}|M)$ is similar to the positive samples $\mathcal{S}_\mathsf{p}^M$ and dissimilar to the negative samples $\mathcal{S}_\mathsf{n}^M$. With similarity measured by dot products, we use an alternative form of InfoNCE (Oord et al., 2018; He et al., 2020), a supervised contrastive loss, that takes into account the solution qualities of both positive and negative samples:

$$\mathcal{L}(\boldsymbol{\theta}) = \sum_{(\mathcal{S}_\mathsf{p}^M, \mathcal{S}_\mathsf{n}^M)\in\mathcal{D}} \frac{-1}{|\mathcal{S}_\mathsf{p}^M|} \sum_{\boldsymbol{x}_\mathsf{p}\in\mathcal{S}_\mathsf{p}^M} l(\boldsymbol{\theta}|\boldsymbol{x}_\mathsf{p}, M)$$

where

$$l(\boldsymbol{\theta}|\boldsymbol{x}_\mathsf{p}, M) = \log \frac{\exp(\boldsymbol{x}_\mathsf{p}^\mathsf{T}\boldsymbol{p}_{\boldsymbol{\theta}}(\boldsymbol{x}_\mathsf{p}|M)/\tau(\boldsymbol{x}_\mathsf{p}|M))}{\sum_{\tilde{\boldsymbol{x}}\in\mathcal{S}_\mathsf{n}^M\cup\{\boldsymbol{x}_\mathsf{p}\}} \exp(\tilde{\boldsymbol{x}}^\mathsf{T}\boldsymbol{p}_{\boldsymbol{\theta}}(\tilde{\boldsymbol{x}}|M)/\tau(\tilde{\boldsymbol{x}}|M))}$$

and we let $\frac{1}{\tau(\boldsymbol{x}|M)} \propto -E(\boldsymbol{x}|M)$ if $\boldsymbol{x}$ is feasible to M where $E(\boldsymbol{x}|M)$ is the same energy function used in previous works (Han et al., 2022; Nair et al., 2020); otherwise $\tau(\boldsymbol{x}|M)$ is set to a constant τ ($\tau = 1$ in experiments). Intuitively, setting $\tau(\boldsymbol{x}|M)$ in this manner encourages the predictions $\boldsymbol{p}_{\boldsymbol{\theta}}(\boldsymbol{x}|M)$ to be more similar to positive samples $\boldsymbol{x}_\mathsf{p}$ with better objectives.

4.3. Predict-and-Search

We apply the predicted solution to reduce the search space of the input MILP the same way as Predict-and-Search (Han et al., 2022). We greedily select $\mathcal{X}_0$ and $\mathcal{X}_1$ based on the prediction and solve the optimization problem defined by Equation (2) given hyperparameters k_0, k_1 and Δ.

5. Empirical Evaluation

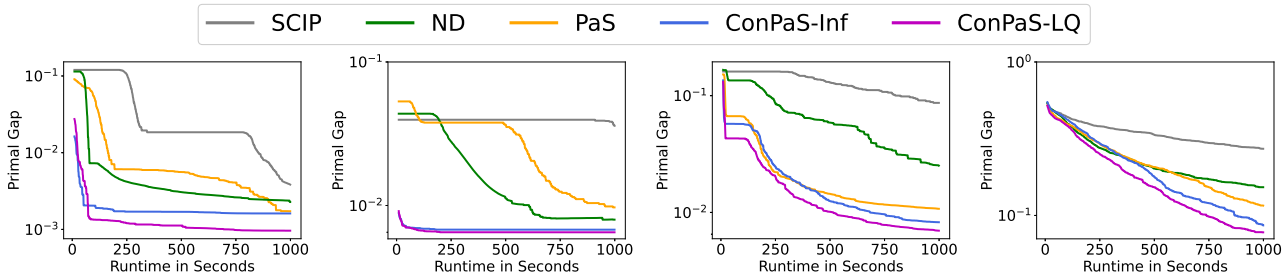
In this section, we introduce the setup for empirical evaluation and then present the results.

5.1. Setup

Benchmark Problems We evaluate on four NP-hard benchmark problems that are widely used in existing studies (Gasse et al., 2019; Han et al., 2022), which consist of two graph optimization problems, namely the minimum vertex cover (MVC) and maximum independent set (MIS) problems, and two non-graph optimization problems, namely the combinatorial auction (CA) and item placement (IP) problems. Both MVC and MIS instances are generated according to the Barabasi-Albert random graph model (Albert & Barabási, 2002), with 6,000 nodes and an average degree of 5. CA instances are generated with 2,000 items and 4,000 bids according to the arbitrary relations in Leyton-Brown et al. (2000). IP instances are provided by the NeurIPS ML4CO competition (Gasse et al., 2022). The workload appointment (WA) problem is another benchmark problem from the competition. However, they are not challenging enough for the baselines and our approach. Therefore, we exclude the results on WA from the main paper and report them in Appendix. For each benchmark problem, we have

Table 1: The average numbers of variables and constraints in the test instances.

Benchmark Problem	MVC	MIS	CA	IP
#Binary Variables	6,000	6,000	4,000	1,050
#Continuous Variables	0	0	0	33
#Constraints	29,975	29,975	2,675	195



(a) MVC (b) MIS (c) CA (d) IP

Figure 2: The primal gap (the lower, the better) as a function of runtime averaged over 100 test instances. ConPaS-LQ and ConPaS-Inf are two variants of ConPaS that use low-quality and infeasible solutions, respectively, as negative samples introduced in Section 4.1.2.

400, 100 and 100 instances in the training, validation and test sets, respectively. For each test set, Table 1 shows its average numbers of variables and constraints. More details of instance generation are included in Appendix.

Baselines We compare ConPaS with three baselines: (1) SCIP (v8.0.1) (Maher et al., 2017), the state-of-the-art open-source ILP solver. We allow restart and presolving with the aggressive mode turned on for primal heuristics to focus on improving the objective value; (2) Neural Diving (ND) (Nair et al., 2020); and (3) Predict-and-Search (PaS) (Han et al., 2022). We have considered another version of PaS where we replace the neural network output with the LP relaxation solutions of the MILP. However, this approach causes very high infeasibility rates when solving the optimization problem defined by Equation (2). We also compare ConPaS with Gurobi (v10.0.0) (Gurobi Optimization, LLC, 2022) and present the results in Appendix.

For ML-based approaches, a separate model is trained for each benchmark problem. For PaS, we train the models with the code by Han et al. (2022). For ND, we implement it and fine-tune its hyperparameters for each problem since their code is not available.

Metrics We use the following metrics to evaluate all approaches: (1) The *primal gap* (Berthold, 2006) is the normalized difference between the primal bound v and a precomputed best known objective value v^*, defined as $\frac{|v-v^*|}{\max(v,v^*,\varepsilon)}$ if v exists and $v \cdot v^* \geq 0$, or 1 otherwise. We use $\varepsilon = 10^{-8}$ to avoid division by zero; v^* is the best primal bound found within 60 minutes by any approach in the portfolio for comparison; (2) The *primal integral* (Achterberg et al., 2012) at runtime cutoff t is the integral on $[0, t]$ of the primal gap as a function of runtime. It captures the quality of the solutions found and the speed at which they are found; and (3) The *survival rate* (Sonnerat et al., 2021) to meet a certain primal gap threshold is the fraction of instances with primal gaps below the threshold.

Hyperparameters We conduct experiments on 2.4 GHz Intel Core i7 CPUs with 16 GB memory. Training is done on a NVIDIA P100 GPU with 32 GB memory. For data collection, we collect 50 best found solutions for each training instance with an hour runtime using Gurobi (v10.0.0). For training, we use the Adam optimizer (Kingma & Ba, 2015) with learning rate 10^{-3}. We use a batch size of 8 and train for 100 epochs (the training typically converges in less than 50 epochs and 5 hours). For testing, we set the runtime cutoff to 1,000 seconds to solve the reduced MILP of each test instance with SCIP (v8.0.1).[2] To tune (k_0, k_1, Δ) (see definition in Section 2.3) for both PaS and ConPaS, we first fix $\Delta = 5$ or 10 and vary k_0, k_1 to be $0\%, 10\%, \ldots, 50\%$ of the number of binary variables to test their performance on the validation set to get their initial values. We then adjust Δ, k_0, k_1 around their initial values to find the best ones. The fine-tuned values are reported in Appendix.

5.2. Results

We test two variants of ConPaS, denoted by ConPaS-Inf and ConPaS-LQ, that use infeasible solutions and low-quality so-

[2]Note that our approach is agnostic to the solver for the reduced MILP. The test results with Gurobi are reported in Appendix.

lutions as negative samples, respectively. Figure 2 shows the primal gap as a function of runtime. Overall, SCIP performs the worst. PaS achieves lower average primal gaps than ND on three of the problems at 1,000 seconds runtime cutoff. Both ConPaS-Inf and ConPaS-LQ show significantly better anytime performance than all baselines on all benchmark problems. ConPaS-LQ performances slightly better than ConPaS-Inf. At the 1,000-second runtime cutoff, ConPaS-Inf achieves 3.54%-52.83% lower average primal gaps and ConPaS-LQ achieves 9.82%-86.02% lower average primal gaps than the best baseline.

Figure 3 shows the survival rate to meet a certain primal gap threshold. The primal gap threshold is chosen as the medium of the average primal gap at 1,000 seconds runtime cutoff among all approaches rounded to the nearest 0.50%. ND surprisingly has the lowest survival rate (even lower than SCIP) on the CA instances, indicating high variance in performance of both SCIP and ND[3], but ND is better than both SCIP and PaS on both the two graph optimization problems. PaS has higher survival rates on the CA and IP instances. ConPaS-Inf and ConPaS-LQ have the best survival rate at 1,000-second runtime cutoff on all instances. Specifically, on the MVC and MIS instances, at the runtime cutoffs when they both first reach 100% survival rates, the best baseline only achieves about 10%-80% survival rates. These results indicate that ConPaS not only finds better solutions on average but also finds them on more instances. Figure 4 shows the average primal integral at 1,000 seconds runtime cutoff. The result demonstrates that both ConPaS-Inf and ConPaS-LQ not only find better solutions than the other approaches but also find them at a faster speed.

Next, we test the generalization performance and conduct an ablation study on the loss functions. Given the large computation overhead, we focus on two representative benchmark problems, a graph optimization problem MVC and a non-graph optimization problem CA.

5.2.1. Generalization to Larger Instances

We test the generalization performance of the trained models on larger instances. We generate 100 large MVC instances according to the Barabasi-Albert random graph model (Albert & Barabási, 2002), with 9,000 nodes and an average degree of 5. We also generate 100 large CA instances with 3,000 items and 6,000 bids according to the arbitrary relations in Leyton-Brown et al. (2000). These larger instances have 50% more variables and constraints than the previous test instances. In Figure 5, we show the results of the average primal gaps, survival rates and the average primal integral over 100 test instances. All ML-based approaches demonstrate good generalizability. On large MVC instances, ND, PaS and ConPaS-Inf perform similarly in terms of the primal gap, while ConPaS-Inf improves the primal gap faster than the other approaches. On large CA instances, both ConPaS-Inf and ConPaS-LQ are significantly better than the other baselines in terms of all performance metrics. Overall, on both large MVC and CA instances, ConPaS-LQ is the best and its primal integral at 1,000 seconds runtime cutoff is 57.9%-70.3% lower than the best baseline PaS. It also reaches 100% survival rates fastest for the given thresholds.

[3]When the primal gap threshold is set to 5.00%, ND has a 98% survival rate whereas SCIP has only 56%.

Table 2: Comparison of different loss functions. We report the primal gaps (PG) and the primal integrals (PI) at the 1,000-second runtime cutoff averaged over 100 instances.

	MVC		CA	
	PG	PI	PG	PI
PaS	0.17%	13.9	1.16%	28.9
ConPaS-LQ-unweighted	0.12%	3.3	0.57%	24.3
ConPaS-LQ	**0.10%**	**2.9**	**0.16%**	**19.7**

5.2.2. Ablation Study

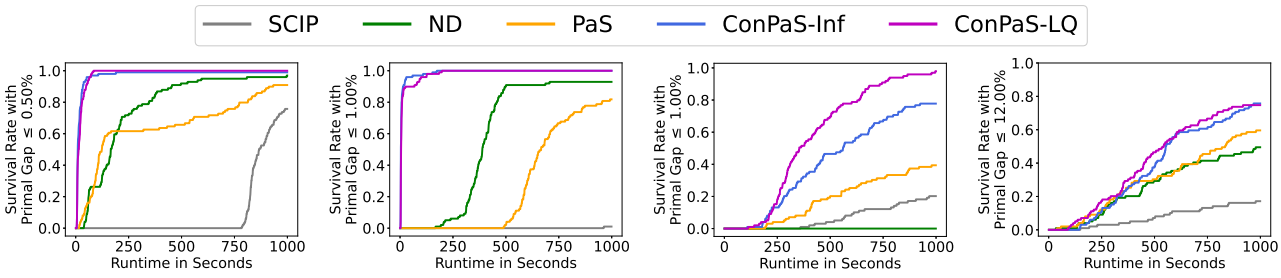
We conduct an ablation study on ConPaS-LQ to assess the effectiveness of the alternate form of InfoNCE loss. The results are shown in Table 2, where ConPaS-LQ-unweighted refers to training using the original InfoNCE loss without considering different qualities of the samples where we fine-tune and set $\tau(\boldsymbol{x}|M)$ to constant 1. ConPaS-LQ refers to the one that takes into account the solution qualities. ConPaS-LQ is still able to outperform PaS. Its performance further improves when the modified loss function is used.

Table 3: The primal gap and primal integral at 1,000 seconds runtime cutoff on the CA instances with different k_0 averaged over 100 instances.

	Primal Gap (%)		Primal Integral	
k_0	PaS	ConPaS-LQ	PaS	ConPaS-LQ
800	6.28	6.59	114.4	117.5
1200	5.45	5.05	104.3	97.3
1600	2.91	2.06	75.6	70.4
2000	1.17	**0.55**	28.9	**19.7**
2400	2.19	1.40	27.5	22.9
2700	5.63	4.58	58.0	47.4
3000	12.74	11.56	127.8	115.8

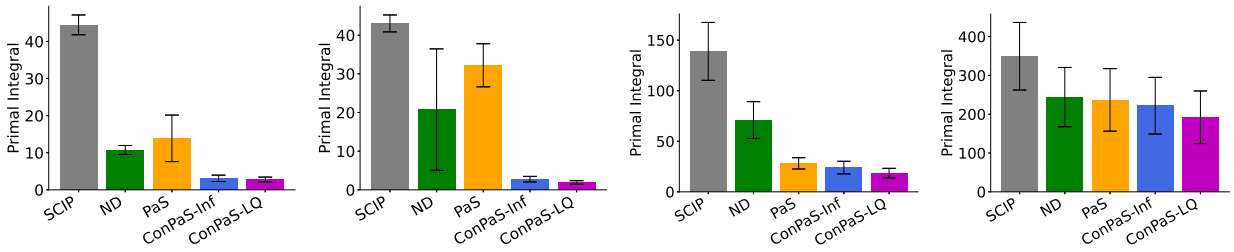
5.2.3. The Effect of Hyperparameters

We study the effect of hyperparameters. Specifically, we focus our study on PaS and ConPaS-LQ on the CA instances. We first empirically study how many training instances are needed for each approach. We train separate models with 50% and 25% of the training instances and test their performance on the test instances. Figure 6 shows the results on the primal gap and primal integral. The two models for ConPaS-LQ trained with 50% and 100% of the instances per-



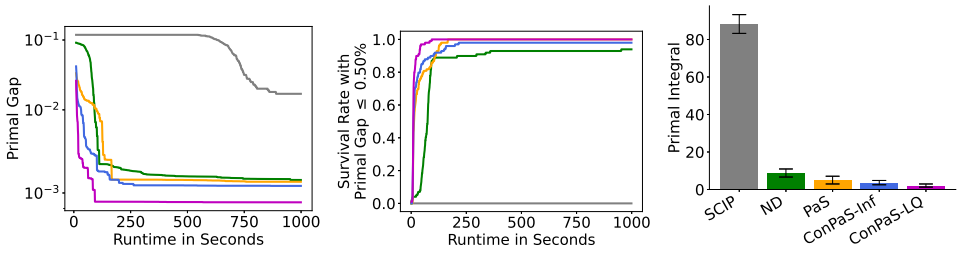
(a) MVC (b) MIS (c) CA (d) IP

Figure 3: The survival rate (the higher, the better) to meet a certain primal gap threshold over 100 test instances as a function of runtime. The primal gap threshold is set to the median of the average primal gaps at 1,000 seconds runtime cutoff among all approaches rounded to the nearest 0.50%.

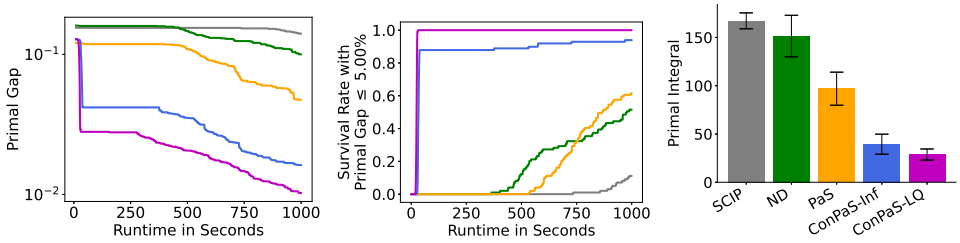


(a) MVC (b) MIS (c) CA (d) IP

Figure 4: The primal integral (the lower, the better) at 1,000 seconds runtime cutoff, averaged over 100 test instances. The error bars represent the standard deviation. A tabular representation is provided in the Appendix Table 6.



(a) MVC (large instances).



(b) CA (large instances).

Figure 5: Generalization to 100 large instances: The primal gap as a function of runtime, the survival rate as a function of runtime and the primal integral at 1,000 seconds runtime cutoff. The primal gap threshold for the survival rate is chosen as the medium of the average primal gaps at 1,000 seconds runtime cutoff among all approaches rounded to the nearest 0.50%. A tabular representation for the primal integral plots is provided in Appendix.

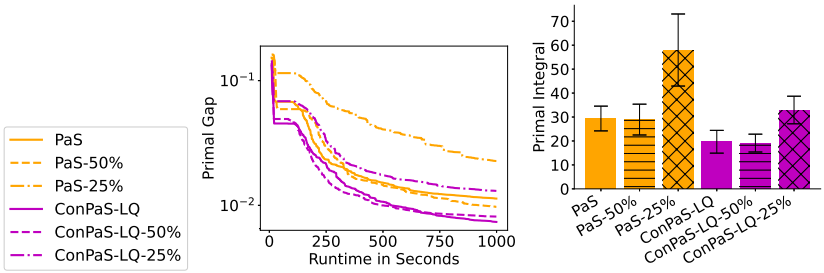


Figure 6: Training on different fractions of training instances: The primal gap as a function of runtime and the primal integral at 1,000 seconds runtime cutoff. ConPaS-LQ-50% and ConPaS-LQ-25% denote the versions of ConPaS trained with only 50% and 25% of the training instances, respectively (similarly for PaS).

form similarly to each other. This is also true for PaS, but its two models are both worse than ConPaS-LQ. When we use 25% of the training instances, we observe a drop in performance for both approaches. However, in this case, ConPaS-LQ performs much better than PaS and only slightly worse than PaS trained on 100% or 50% instances. These empirical results indicate that CL can achieve better performance using fewer training instances than other learning approaches.

We also study the effect of different (k_0, k_1, Δ) for PaS and ConPaS-LQ on the CA instances. For CA instances, fixing both k_1 and Δ to 0 always gives better primal gaps and primal integrals than other values. Therefore, we vary only k_0. We present the results on primal gaps and primal integrals in Table 5. Overall, setting $k_0 = 2,000$ gives the best performance for both PaS and ConPaS-LQ. Either increasing or decreasing k_0 from 2,000 hurts their performance. However, if we increase k_0 from 2,000, both of them converge to the eventual solutions fast and therefore have comparable primal integrals with small k_0, even though sometimes their primal gaps are worse. In general, having a smaller k requires the search to search for the values on more variables; therefore, it converges slower and has a larger primal integral. On the other hand, having a larger k reduces the search space more, therefore, it converges faster but to a worse solution.

6. Conclusion

We proposed ConPaS, a contrastive predict-and-search framework for MILPs. We learned to predict high-quality solutions by contrasting optimal and near-optimal solutions with infeasible or low-quality solutions. In testing, we solved a reduced MILP by restricting the search space to proximity to the predicted solutions. In experiments, we showed that ConPaS found solutions better and faster than the baselines, which include two state-of-the-art ML-based approaches. ConPaS also demonstrated generalizability to larger instances that were unseen during training. Solving MILPs based on solution predictions, such as ConPaS, ND and PaS, does not guarantee completeness or optimality. The contrastive-learned model in ConPaS can be used in different ways, e.g., setting branching priority in Branch-and-Cut. We believe it is important and interesting for future work to integrate it into optimal tree searches.

Impact Statement

This paper presents work whose goal is to advance the field of machine learning for combinatorial optimization. There are many potential societal consequences of our work, none of which we feel must be specifically highlighted here.

Acknowledgments

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Appendix

A. GCN Architecture

We follow previous work (Gasse et al., 2019; Han et al., 2022) to use a bipartite graph representation to encode a MILP M. For the node (variable and constraint)and edge features of the bipartite graph, we use the same features as (Han et al., 2022).

We use the same GCN architecture as previous work (Han et al., 2022). The GCN takes as input the bipartite graph representation of a MILP M with its features and outputs $\boldsymbol{p}_{\boldsymbol{\theta}}(\boldsymbol{x}|M)$, a $[0, 1]$-score vector for the binary variables. For node features, we use 2-layer multi-layer perceptrons (MLP) with 64 hidden units per layer and ReLU as the activation function to map them to $\mathbb{R}^{64}$. We then perform two rounds of message-passings, the first one from variable nodes to constraint nodes and the second one from constraint nodes to variable nodes, using graph convolution layers (Gasse et al., 2019) to obtain a final variable embedding. The final variable embedding is then passed through a 2-layer MLP with 64 hidden units per layer and ReLU as the activation function followed by a sigmoid layer to obtain the output $\boldsymbol{p}_{\boldsymbol{\theta}}(\boldsymbol{x}|M)$.

B. Benchmark Problem Descriptions and MILP Formulations

We present the problem descriptions and MILP formulations for the minimum vertex cover (MVC), maximum independent set (MIS) and combinatorial auction (CA) problems. The descriptions and formulations for the item placement and workload appointment problems can be found at the ML4CO competition (Gasse et al., 2022) website[4].

In the MVC problem, given an undirected graph $G = (V, E)$ with a weight w_v associated with each node $v \in V$, we want to select a subset of nodes $V' \subseteq V$ with the minimum sum of weights such that at least one endpoint of the edge is selected in V' for any edge in E:

$$\begin{aligned} &\min \textstyle\sum_{v\in V} w_v x_v \\ \text{s.t.} \quad &x_u + x_v \geq 1, \forall (u, v) \in E, \\ &x_v \in \{0, 1\}, \forall v \in V. \end{aligned}$$

In the MIS problem, given an undirected graph $G = (V, E)$, we want to select the largest subset of nodes $V' \subseteq V$ such that no two nodes in the subsets are connected by an edge in G:

$$\begin{aligned} &\min -\textstyle\sum_{v\in V} x_v \\ \text{s.t.} \quad &x_u + x_v \leq 1, \forall (u, v) \in E, \\ &x_v \in \{0, 1\}, \forall v \in V. \end{aligned}$$

In the CA problem, given n bids $\{(B_i, p_i) : i \in [n]\}$ for m items, where B_i is a subset of items and p_i is the bidding price for B_i, we want to allocate items to bids such that the total revenue is maximized:

$$\begin{aligned} &\min -\textstyle\sum_{i\in[n]} p_i x_i \\ \text{s.t.} \quad &\textstyle\sum_{i:j\in B_i} x_i \leq 1, \forall j \in [m], \\ &x_i \in \{0, 1\}, \forall i \in [n]. \end{aligned}$$

C. Hyperparameters

In this section, we discuss the hyperparameters used for SCIP, ND, PaS and ConPaS.

For SCIP, we fine-tune its restart, presolving and primal heuristic modes on the validation instances. We observe that allowing both restarts and presolving with the aggressive mode turned on for primal heuristics yields the best performance for SCIP. For SCIP with the default mode, it delivers similar primal performance for the CA problem but is worse than the fine-tuned version on others. We also observe that allowing restarts is especially helpful for the IP problem.

For ND, following Nair et al. (2020), we train a model separately for each coverage rate value. Due to limited computing resources, we train models with coverage rate values in $\{0.2, 0.3, 0.4\}$. The best coverage rates we found for the MVC, MIS, CA and IP problems are 0.2, 0.2, 0.4 and 0.3, respectively.

[4]ML4CO Competition Website: https://github.com/ds4dm/ml4co-competition/blob/main/DATA.md

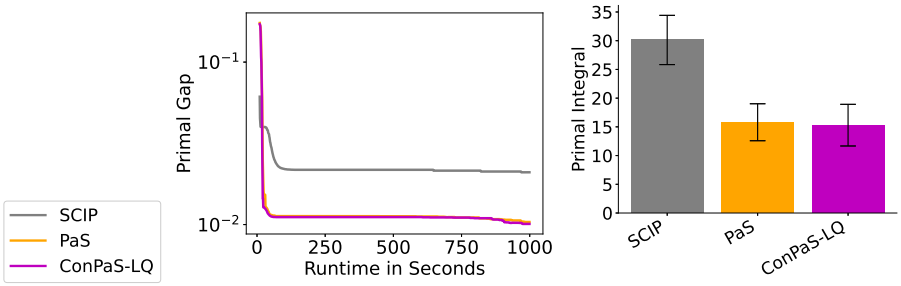


Figure 7: The primal gap as a function of runtime and the primal integral at 1,000 seconds runtime cutoff. Note that the curves of PaS and ConPaS highly overlap with each other.

Table 4: Hyperparameters (k_0, k_1, Δ) used for PaS and ConPaS.

	PaS	ConPaS-Inf	ConPaS-LQ
MVC	$(500, 100, 10)$	$(800, 200, 20)$	$(800, 200, 20)$
MIS	$(600, 600, 5)$	$(1200, 600, 10)$	$(1000, 600, 15)$
CA	$(2000, 0, 0)$	$(2000, 0, 0)$	$(2000, 0, 0)$
IP	$(400, 5, 3)$	$(400, 5, 5)$	$(400, 5, 2)$

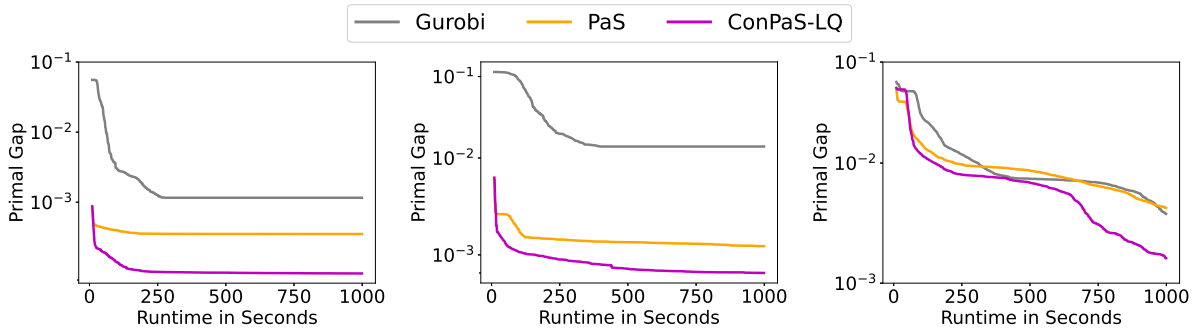
For PaS and ConPaS, the values of k_0, k_1 and Δ are summarized in Table 4. Note that the best hyperparameters for both MVC and MIS are quite different for PaS and ConPaS. On MVC instances for PaS, we observe that $(k_0, k_1, \Delta) = (600, 200, 20)$ has a smaller primal integral than $(500, 100, 10)$ but has a larger primal gap at 1,000 seconds runtime cutoff. We also test $(k_0, k_1, \Delta) = (500, 100, 10)$ for ConPaS-LQ, it converges to the same primal gaps (with $< 0.002\%$ differences) as $(800, 200, 20)$ but has a 34.1% increase in primal integral. On MIS instances for PaS, we observe that increasing k_0 or Δ (or both) leads to significantly worse performance. However, if we use $(k_0, k_1, \Delta) = (600, 600, 6)$ for ConPaS-LQ, it converges to the same primal gaps (with $< 0.032\%$ differences) as $(1000, 600, 15)$ but has a 131.8% increase in primal integral (still being better than any other baseline).

Table 5: The primal gap and primal integral at 1,000 seconds runtime cutoff on the CA instances with different k_0 averaged over 100 instances.

	Primal Gap (%)		Primal Integral	
k_0	PaS	ConPaS-LQ	PaS	ConPaS-LQ
800	6.28	6.59	114.4	117.5
1200	5.45	5.05	104.3	97.3
1600	2.91	2.06	75.6	70.4
2000	1.17	**0.55**	28.9	**19.7**
2400	2.19	1.40	27.5	22.9
2700	5.63	4.58	58.0	47.4
3000	12.74	11.56	127.8	115.8

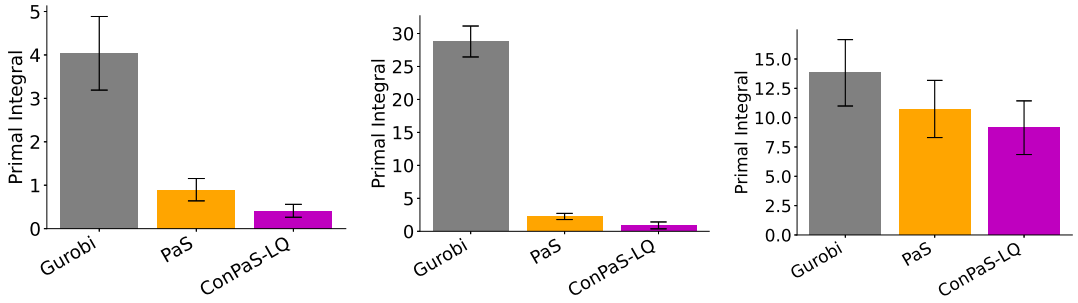
Table 6: Tabular representation of the primal integral plots in Figures 4 and 5: The primal integral and the standard deviation at 1,000 seconds runtime cutoff, averaged over 100 instances.

	SCIP	ND	PaS	ConPaS-Inf	ConPaS-LQ
MVC	44.5±2.7	10.7±1.2	13.9±6.3	3.1±0.9	**2.8±0.6**
MIS	46.3±2.9	22.9±14.9	34.5±5.8	5.5±1.3	**5.4±1.3**
CA	138.9±28.6	71.0±18.2	28.9±5.6	24.0±6.2	**19.7±4.8**
IP	349.3±87.1	244.0±76.4	236.8±80.6	221.8±73.0	**192.0±67.8**
MVC (large)	88.3±5.0	8.8±2.2	5.0±2.1	3.7±1.1	**2.1±0.8**
CA (large)	167.2±8.2	151.4±21.5	96.9±17.1	39.4±10.4	**28.7±5.7**



(a) MVC. (b) MIS. (c) CA.

Figure 8: Comparisons with Gurobi: The primal gap (the lower, the better) as a function of runtime averaged over 100 test instances.



(a) MVC. (b) MIS. (c) CA.

Figure 9: Comparisons with Gurobi: The primal integral (the lower, the better) at 1,000 seconds runtime cutoff, averaged over 100 test instances. The error bars represent the standard deviation.

D. Additional Experimental Results

D.1. Results on the Workload Appointment Problem

Figure 7 presents the results on the WA instances. Both PaS and ConPaS-LQ outperform SCIP significantly in terms of the primal gap and the primal integral. However, both approaches converge quickly to low primal gaps, with ConPaS-LQ being very slightly better than PaS.

D.2. Comparisons with Gurobi

We compare the performance of ConPaS-LQ against PaS and Gurobi on the MVC, MIS and CA instances. Note that in this experiment, we use Gurobi in the Predict-and-Search phase for both PaS and ConPaS-LQ to ensure a fair comparison. The hyperparameters (k_0, k_1, Δ) are reported in Table 7. Figure 8 shows the primal gap as a function of runtime. Figure 9 shows the primal integral at 1,000 seconds runtime cutoff. The results show that both PaS and ConPaS-LQ outperform Gurobi significantly on MVC and MIS instances. Overall, ConPaS-LQ is still the best when applied on Gurobi.

D.3. Prediction Accuracy

To assess the accuracy of the predicted solutions by the neural networks, we report the classification accuracy over all binary variables (with the threshold set to 0.5) in Table 8. We report it for both PaS and ConPaS-LQ on the MVC and CA problems on 100 validation instances. The accuracy is the fraction of correctly classified variables averaged over 50 positive samples for each instance, and we report the average accuracy over 100 validation instances. Since the classification accuracy is sensitive to the threshold, we also report the AUROC. On the MVC instances, though ConPaS has a lower accuracy (w.r.t. the threshold of 0.5), it has higher AUROC than PaS. On the CA instances, their accuracies and AUROCs are similar.

Table 7: Comparisons with Gurobi: Hyperparameters (k_0, k_1, Δ) used for PaS and ConPaS-LQ.

	PaS	ConPaS-LQ
MVC	$(500, 100, 10)$	$(500, 100, 15)$
MIS	$(500, 500, 10)$	$(500, 500, 10)$
CA	$(1500, 0, 0)$	$(1500, 0, 0)$

Table 8: Prediction accuracy and AUROC on 100 validation instances.

	MVC		CA	
	Accuracy	AUROC	Accuracy	AUROC
PaS	81.2%	0.88	88.3%	0.87
ConPaS-LQ	76.9%	0.91	86.9%	0.86

However, we would like to point out that a better accuracy/AUROC does not necessarily indicate a better downstream search performance.