SurCo: Learning Linear SURrogates for COMbinatorial Nonlinear Optimization Problems

Anonymous authors
Paper under double-blind review

Abstract

Optimization problems with expensive nonlinear cost functions and combinatorial constraints appear in many real-world applications, but remain challenging to solve efficiently. Existing combinatorial solvers like Mixed Integer Linear Programming can be fast in practice but cannot readily optimize nonlinear cost functions, while general nonlinear optimizers like gradient descent often do not handle complex combinatorial structures, may require many queries of the cost function, and are prone to local optima. To bridge this gap, we propose ***SurCo*** that learns linear Surrogate costs which can be used by existing Combinatorial solvers to output good solutions to the original nonlinear combinatorial optimization problem, combining the flexibility of gradient-based methods with the structure of linear combinatorial optimization. We learn these linear surrogates end-to-end with the nonlinear loss by differentiating through the linear surrogate solver. Three variants of SurCo are proposed: SurCo-zero operates on individual nonlinear problems, SurCo-prior trains a linear surrogate predictor on distributions of problems, and SurCo-hybrid uses a model trained offline to warm start online solving for SurCo-zero. We analyze our method theoretically and empirically, showing smooth convergence and improved performance. Experiments show that compared to state-of-the-art approaches and expert-designed heuristics, SurCo obtains lower cost solutions with comparable or faster solve time for two real-world industry-level applications: embedding table sharding and inverse photonic design.

1 Introduction

Combinatorial optimization problems with linear objective functions, like linear programming (LP) (Chvatal et al., 1983) and mixed integer linear programming (MILP) (Wolsey, 2007), have been extensively studied in operations research (OR). The resulting high-performance solvers like Gurobi (Gurobi Optimization, LLC, 2022) can solve industrial-scale optimization problems with ten of thousands of variables in a few minutes.

However, even with perfect solvers, one issue remains: the cost functions $f(\boldsymbol{x})$ in many practical problems are *nonlinear*, and the highly-optimized solvers mainly handle linear or convex formulations while real-world problems have less constrained objectives. For example, in embedding table sharding (Zha et al., 2022a) one needs to distribute embedding tables to multiple GPUs for the deployment of recommendation systems. Due to the batching behaviors within a single GPU and communication cost among different GPUs, the overall latency (cost function) in this application depends on interactions of multiple tables and thus can be highly nonlinear (Zha et al., 2022a).

To obtain useful solutions to the real-world problems, one may choose to directly optimize the nonlinear cost, which is either a black-box output of a simulator (Gosavi et al., 2015; Ye et al., 2019), or a cost estimator learned by machine learning techniques (e.g., deep models) from offline data (Steiner et al., 2021; Koziel et al., 2021; Wang et al., 2021b; Cozad et al., 2014). However, many of these direct optimization approaches either rely on human-defined heuristics (e.g., greedy (Korte & Hausmann, 1978; Reingold & Tarjan, 1981; Wolsey, 1982), local improvement (Voß et al., 2012; Li et al., 2021)), or resort to general nonlinear optimization techniques like gradient descent (Ruder, 2016), reinforcement learning (Mazyavkina et al., 2021), or evolutionary algorithms (Simon, 2013). While these approaches can work in practice, they may lead to a slow optimization process, in particular when the cost function is expensive to evaluate, and they often ignore the combinatorial nature of most real-world applications (encoded in the feasible set $\boldsymbol{x} \in \Omega$).

In this work, we propose a systematic framework ***SurCo*** that leverages existing efficient combinatorial solvers to find solutions to nonlinear combinatorial optimization problems arising in real-world scenarios. There are three versions of SurCo, SurCo-zero, SurCo-prior, and SurCo-hybrid. In SurCo-zero, given a nonlinear *differentiable* cost $f(\boldsymbol{x})$ to be minimized, we optimize a *linear surrogate* cost $\hat{\boldsymbol{c}}$ so that the *surrogate optimizer* (SO) $\min_{\boldsymbol{x}\in\Omega} \hat{\boldsymbol{c}}^\top \boldsymbol{x}$ outputs a solution that is expected to be optimal w.r.t. the *original* nonlinear cost $f(\boldsymbol{x})$. Due to its linear nature, SO can be solved efficiently with existing solvers, and the surrogate cost $\hat{\boldsymbol{c}}$ can be optimized in an end-to-end manner by back-propagating *through* the solver (Pogančić et al., 2019; Niepert et al., 2021; Berthet et al., 2020). In SurCo-prior, we consider a family of nonlinear differentiable functions $f(\boldsymbol{x};\boldsymbol{y})$, where $\boldsymbol{y}$ parameterizes problem descriptions. We train the linear surrogate $\hat{\boldsymbol{c}}(\boldsymbol{y})$ on a set of optimization problems (called the training set $\{\boldsymbol{y}_i\}$), and evaluate on a held-out problem $\boldsymbol{y}'$, by directly optimizing SO: $\boldsymbol{x}^*(\boldsymbol{y}') := \arg\min_{\boldsymbol{x}\in\Omega(\boldsymbol{y})} \hat{\boldsymbol{c}}^\top(\boldsymbol{y}')\boldsymbol{x}$, which avoids optimizing the cost $f(\boldsymbol{x};\boldsymbol{y}')$ from scratch. Finally, in SurCo-hybrid we use initial surrogate costs predicted by a fully-trained SurCo-prior and then fine-tune the surrogate costs further using SurCo-zero to leverage both domain knowledge synthesized offline and information about the specific instance.

All versions of SurCo are evaluated in two real-world nonlinear optimization problems: embedding table sharding (Zha et al., 2022a), and photonic inverse design (Schubert et al., 2022). In both cases, we show that in the on-the-fly setting, SurCo achieves higher quality solutions in comparable or less runtime, faster optimization in wall-clock time with lower solution cost, thanks to the help of an efficient combinatorial solver; in prior, our method obtains better solutions in held-out problems compared to other methods that require training (e.g., reinforcement learning). More specifically, in table sharding SurCo-zero obtains between 14% to 85% improvement in solution quality with between 2% and 23% increase in runtime overhead compared to the greedy baseline, SurCo-prior obtains between 47% and 71% solution quality improvement against the state of the art RL-based table sharding algorithm Zha et al. (2022b). SurCo-hybrid obtains better solutions than either SurCo-zero or SurCo-prior, with a similar runtime overhead as SurCo-zero. In photonic inverse design, SurCo-zero finds 21% more viable solutions for the beam splitter and twice as many solutions for the wavelength demultiplexers with all problems solving successfully for the mode converter and bend problems, taking between 10% to 64% less time than the pass-through approach from previous work (Schubert et al., 2022). While the offline trained SurCo-prior misses some optimal solutions in the different settings, it frequently obtains solutions in 0.5% to 2% of the runtime due to not needing to evaluate the objective and perform gradient steps. Again, SurCo-hybrid is able to obtain solutions more often than the other approaches, with a runtime overhead comparable to SurCo-zero. We additionally present theoretical results that help motivate why training a model to predict surrogate linear coefficients exhibits better sample complexity than directly predicting the optimal solution (Li et al., 2018; Ban & Rudin, 2019).

2 Problem Specification

Our goal is to solve the following nonlinear optimization problem describe by $\boldsymbol{y}$:

$$\min_{\boldsymbol{x}} f(\boldsymbol{x};\boldsymbol{y}) \qquad \text{s.t.} \quad \boldsymbol{x} \in \Omega(\boldsymbol{y}) \tag{1}$$

where $\boldsymbol{x} \in \mathbb{R}^n$ are the variables to be optimized, $f(\boldsymbol{x};\boldsymbol{y})$ is the nonlinear differentiable cost function to be minimized, $\Omega(\boldsymbol{y})$ is the feasible region, typically specified by linear (in)equalities and integer constraints, and $\boldsymbol{y} \in Y$ are the problem instance parameters drawn from a distribution $\mathcal{D}$ over Y. For example, in the traveling salesman problem, $\boldsymbol{y}$ can be the distance matrix among cities. We often consider solving a family of optimization problems, described as $\boldsymbol{y} \in Y$.

Differentiable cost function. The nonlinear cost function $f(\boldsymbol{x};\boldsymbol{y})$ can either be the result of a simulator made differentiable via finite differencing (e.g., JAX (Bradbury et al., 2018)), or a cost model that is learned from an offline dataset, often generated via sampling multiple feasible solutions within $\Omega(\boldsymbol{y})$, and recording their costs. The cost model often takes the form of a deep neural network. In this work, we assume the following property of $f(\boldsymbol{x};\boldsymbol{y})$:

Assumption 2.1 (Cost function). *During optimization, the cost function $f(\boldsymbol{x};\boldsymbol{y})$ and its partial derivative $\partial f/\partial \boldsymbol{x}$ are accessible.*

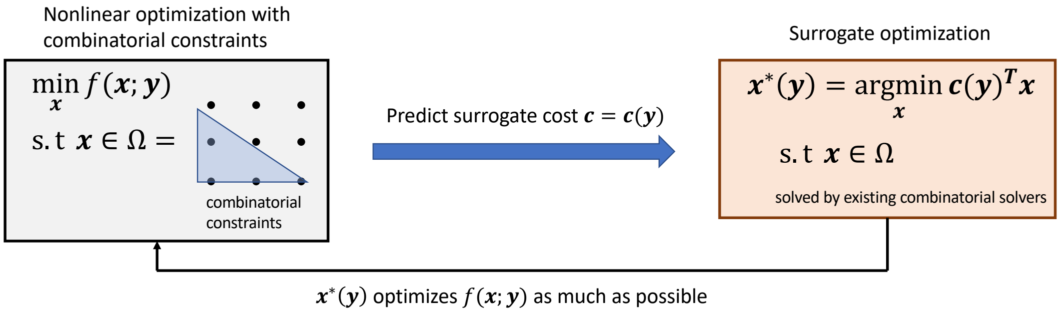


Figure 1: Overview of our proposed algorithm SurCo.

Learning a good nonlinear cost model f is highly non-trivial for practical applications (e.g., AlphaFold (Jumper et al., 2021), Density Functional Theory (Nagai et al., 2020), cost model for embedding tables (Zha et al., 2022a)) and is beyond the scope of this work.

Evaluation Metric. In real-world applications, querying f can be slow and expensive, and thus a lower number of queries while getting better quality solution is the goal. We mainly focus on two aspects: how good the solution $\hat{\boldsymbol{x}}$ is, by checking the value of $f(\hat{\boldsymbol{x}}; \boldsymbol{y})$, and how many queries of the nonlinear function f are needed during optimization in order to achieve the solution $\hat{\boldsymbol{x}}$.

Linear/nonlinear cost function. When $f(\boldsymbol{x}; \boldsymbol{y})$ is linear w.r.t $\boldsymbol{x}$, and the feasible region can be encoded using mixed integer programs or other mathematical programs, the problem can be solved efficiently using existing scalable optimization solvers. When $f(\boldsymbol{x}; \boldsymbol{y})$ is nonlinear, we propose SurCo that learns a surrogate linear objective function, which allow us to leverage these existing scalable optimization solvers, and which results in a solution that has high quality with respect to the original hard-to-encode objective function $f(\boldsymbol{x}; \boldsymbol{y})$. We will elaborate in the following sections.

3 SurCo: Learning Linear Surrogates

3.1 SurCo-zero: On-the-fly Optimization

We start from the simplest case in which we focus on a single instance with $f(\boldsymbol{x}) = f(\boldsymbol{x}; \boldsymbol{y})$ and $\Omega = \Omega(\boldsymbol{y})$. SurCo-zero aims to optimize the following objective:

$$\text{(SurCo-zero)}: \quad \min_{\boldsymbol{c}} \mathcal{L}_{\text{zero}}(\boldsymbol{c}) := f(\boldsymbol{g}_\Omega(\boldsymbol{c})) \tag{2}$$

where the surrogate optimizer $\boldsymbol{g}_\Omega : \mathbb{R}^n \mapsto \mathbb{R}^n$ is the output of certain combinatorial solvers with linear cost weight $\boldsymbol{c} \in \mathbb{R}^n$ and feasible region $\Omega \subseteq \mathbb{R}^n$. For example, $\boldsymbol{g}_\Omega$ can be the following (n is the number of variables to be optimized):

$$\boldsymbol{g}_\Omega(\boldsymbol{c}) := \arg\min_{\boldsymbol{x}} \boldsymbol{c}^\top \boldsymbol{x} \quad \text{s.t.} \ \ \boldsymbol{x} \in \Omega := \{A\boldsymbol{x} \leq \boldsymbol{b}, \boldsymbol{x} \in \mathbb{Z}^n\} \tag{3}$$

which is the output of a MILP solver. Thanks to previous works (Ferber et al., 2020; Pogančić et al., 2019), we can efficiently compute the partial derivative $\partial \boldsymbol{g}_\Omega(\boldsymbol{c})/\partial \boldsymbol{c}$. Intuitively, this means that $\boldsymbol{g}_\Omega(\boldsymbol{c})$ can be *backpropagated* through.

Since f is also differentiable with respect to the solution it is evaluating, we thus can optimize Eqn. 2 in an end-to-end manner using any gradient-based optimizer. That is, $\boldsymbol{c}(t+1) = \boldsymbol{c}(t) - \alpha \frac{\partial \boldsymbol{g}_\Omega}{\partial \boldsymbol{c}} \frac{\partial f}{\partial \boldsymbol{x}}$, where α is the learning rate. The procedure starts from a randomly initialized $\boldsymbol{c}(0)$ and converges at a local optimal solution of $\boldsymbol{c}$.

While Eqn. 2 is still nonlinear optimization and there is no guarantee about the quality of the final solution $\boldsymbol{c}$, we argue that optimizing Eqn. 2 is better than optimizing the original nonlinear cost $\min_{\boldsymbol{x}\in\Omega} f(\boldsymbol{x})$. Furthermore, while we cannot guarantee optimality, we are able to guarantee feasibility by leveraging a linear combinatorial solver. Intuitively, instead of optimizing directly over the solution space $\boldsymbol{x}$, we optimize over the space of surrogate costs $\boldsymbol{c}$, and delegate the combinatorial feasibility requirements of the nonlinear problem to SoTA combinatorial solvers. Compared to naive approaches that directly optimize $f(\boldsymbol{x})$ via general optimization techniques, our method readily handles complex constraints of the feasible regions, and thus makes the optimization procedure easier.

Furthermore, it also helps escape from local minima, thanks to the embedded search component of existing combinatorial solvers (e.g., branch-and-bound (Land & Doig, 2010) in MILP solvers). As we see in the experiments, this is particularly important when the problem becomes large-scale with more local optima. This approach works well when we are optimizing individual instances and may not have access to offline training data or the training time is cost-prohibitive.

3.2 SurCo-prior: Offline surrogate training

We now discuss more general cases, where the nonlinear loss function $f(\boldsymbol{x};\boldsymbol{y})$ represents *a family* of cost function to be optimized. Here the description of each *problem instance* $\boldsymbol{y}$ is drawn from a fixed problem distribution $\mathcal{D}$. We then ask the following question: how can we find solutions to a batch of training instances $\mathcal{D}_{\text{train}} := \{\boldsymbol{y}_i\}_{i=1}^N$, gain useful knowledge of the cost functions, and leverage such knowledge in held-out evaluation problem instances $\mathcal{D}_{\text{eval}}$ to accelerate the optimization procedure?

Following standard machine learning practice, let us first consider a naive two-stage approach. In the data collection stage, we simply apply `SurCo-zero`(Eqn. 2) to every $\boldsymbol{y}_i$ separately to get N surrogate cost vectors $\boldsymbol{c}_i$. Then in the training stage, we train a regressor $\hat{\boldsymbol{c}} = \hat{\boldsymbol{c}}(\boldsymbol{y};\boldsymbol{\theta})$ on the dataset $\{(\boldsymbol{y}_i, \boldsymbol{c}_i)\}$ to learn to predict the surrogate costs from the problem features. Here $\hat{\boldsymbol{c}}$ is a parameterized model (e.g., a deep network) with the parameters $\boldsymbol{\theta}$ to be learned. This learned regressor $\hat{\boldsymbol{c}}(\boldsymbol{y};\boldsymbol{\theta})$ can thus be used for a held-out problem instance $\boldsymbol{y}'$ to directly predict $\boldsymbol{c}' = \hat{\boldsymbol{c}}(\boldsymbol{y}';\boldsymbol{\theta})$ and get the solution $\boldsymbol{x}' = \boldsymbol{g}_{\Omega(\boldsymbol{y}')}(\boldsymbol{c}')$ via surrogate optimizer (SO).

While this approach is simple, the N optimization procedures in the data collection stage are independent of each other, and can lead to excessive number of calls to f that are not helpful. E.g., if an optimization procedure converges to a bad local solution, then even if it achieves perfect convergence, which requires a lot of function calls, the resulting data point is still of low quality.

This motivates us to add a *regularizer* for the optimization:

$$(\texttt{SurCo-prior-}\lambda): \quad \min_{\boldsymbol{\theta},\{\boldsymbol{c}_i\}} \mathcal{L}_{\texttt{prior}}(\boldsymbol{\theta},\{\boldsymbol{c}_i\};\lambda) := \sum_{i=1}^N f(\boldsymbol{g}_{\Omega(\boldsymbol{y}_i)}(\boldsymbol{c}_i);\boldsymbol{y}_i) + \lambda\|\boldsymbol{c}_i - \hat{\boldsymbol{c}}(\boldsymbol{y}_i;\boldsymbol{\theta}))\|_2 \tag{4}$$

Note that when $\lambda = 0$, it reduces to N independent optimizations, while when $\lambda > 0$, the surrogate costs $\{\boldsymbol{c}_i\}$ interact with each other. The intuition is that, the regressor $\hat{c}(\boldsymbol{y};\boldsymbol{\theta})$, even if not trained fully, can be very useful to guide $\boldsymbol{c}_i$ rather than just using its randomly initialized version. Furthermore, if $\hat{\boldsymbol{c}}$ is a mapping to global optimal solution of $\boldsymbol{c}$, then it will pull the solutions out of local optima to re-target towards global ones, even when starting from poor initialization, yielding fast convergence and better final solutions for individual optimization instances.

A special case is when $\lambda \to +\infty$, we arrive at a novel objective that jointly learns the surrogate cost function, given the training set $\mathcal{D}_{\text{train}}$:

$$(\texttt{SurCo-prior}): \quad \min_{\boldsymbol{\theta}} \mathcal{L}_{\texttt{prior}}(\boldsymbol{\theta}) := \sum_{i=1}^N f(\boldsymbol{g}_{\Omega(\boldsymbol{y}_i)}(\hat{\boldsymbol{c}}(\boldsymbol{y}_i;\boldsymbol{\theta}));\boldsymbol{y}_i) \tag{5}$$

This approach is useful when the goal is to find high-quality solutions for unseen instances of a problem distribution when the upfront cost of offline training is acceptable but the cost of optimizing on-the-fly is prohibitive. Here, we require access to a distribution of training optimization problems, but at test time only require the feasible region and not the nonlinear objective.

3.3 SurCo-hybrid: Fine-tuning a predicted surrogate

Naturally, we consider `SurCo-hybrid`, a hybrid approach which initializes the coefficients of `SurCo-zero` with the coefficients predicted from `SurCo-prior` which was trained on offline data. This allows `SurCo-hybrid` to start out optimization from an initial prediction which has good performance for the distribution at large but which is then fine-tuned for the specific instance. Formally, we initialize $\boldsymbol{c}(0) = \hat{\boldsymbol{c}}(\boldsymbol{y}_i;\boldsymbol{\theta})$ and then continue optimizing $\boldsymbol{c}$ based on the update from `SurCo-zero`. This approach is geared towards optimizing the nonlinear objective using a high-quality initial prediction that is based on the problem distribution and then fine-tuning the objective coefficients based on the specific problem instance at test time. Here, high performance comes at the runtime cost of both having to train offline on a problem distribution as well as performing fine-tuning steps on-the-fly. However, this additional cost is often worthwhile when the main goal is to find the best possible solutions by leveraging synthesized domain knowledge in combination with individual problem instances as arises in chip design (Mirhoseini et al., 2021) and compiler optimization (Zhou et al., 2020).

3.4 Cost Regression versus Solution Regression: A Theoretical Analysis

We also want to compare `SurCo` with the previous works on ML optimizers (Ban & Rudin, 2019) that try to directly learn the mapping from problem description $\boldsymbol{y}$ to the solution, i.e. solution regression. Given a set of training instances $\mathcal{D}_{\mathrm{train}}$ from distribution $\mathcal{D}$, these approaches first collect a set of training samples $\mathcal{D}_{\mathrm{direct}} := \{\boldsymbol{y}, \boldsymbol{x}^*(\boldsymbol{y}) : \boldsymbol{y} \in \mathcal{D}_{\mathrm{train}}\}$, and then learn a function $\tilde{\boldsymbol{x}}^*(\boldsymbol{y})$ to fit the training samples.

While this is conceptually simple, there exist fundamental difficulties to learn such a direct mapping. First, as mentioned above, it can be quite expensive to obtain the optimal solution $\boldsymbol{x}^*(\boldsymbol{y})$ due to the nature of nonlinear optimization and the query cost. Second, even if a perfect dataset $\mathcal{D}_{\mathrm{direct}}$ is accessible, the number of samples needed to learn a mapping to directly predict $\boldsymbol{x}^*(\boldsymbol{y})$ is related to the *Lipschitz constant* L of the mapping, and for a direct mapping, L can be very large.

3.4.1 Lipschitz constant and sample complexity

Let us first consider the sample complexity of solution regression methods as described above.

Formally, consider fitting any function $\boldsymbol{\phi} : \mathbb{R}^d \supseteq Y \mapsto \mathbb{R}^m$ with a dataset $\{\boldsymbol{y}_i, \boldsymbol{\phi}_i\}$. Here Y is a compact region with finite volume $\mathrm{vol}(Y)$. The Lipschitz constant L is the smallest number so that $\|\boldsymbol{\phi}(\boldsymbol{y}_1) - \boldsymbol{\phi}(\boldsymbol{y}_2)\|_2 \le L\|\boldsymbol{y}_1 - \boldsymbol{y}_2\|_2$ holds for any $\boldsymbol{y}_1, \boldsymbol{y}_2 \in Y$. The following theorem shows that if the dataset covers the space Y, we could achieve high accuracy prediction: $\|\boldsymbol{\phi}(\boldsymbol{y}) - \hat{\boldsymbol{\phi}}(\boldsymbol{y})\|_2 \le \epsilon$ for any $\boldsymbol{y} \in Y$.

Definition 3.1 (δ-cover). *A dataset $\mathcal{D}_{\mathrm{direct}} := \{(\boldsymbol{y}_i, \boldsymbol{\phi}_i)\}_{i=1}^N$ δ-covers the space Y, if for any $\boldsymbol{y} \in Y$, there exists at least one $\boldsymbol{y}_i$ so that $\|\boldsymbol{y} - \boldsymbol{y}_i\|_2 \le \delta$.*

Lemma 3.1 (Sufficient condition of prediction with ϵ-accuracy). *If the dataset $\mathcal{D}_{\mathrm{direct}}$ (ϵ/L)-cover Y, then for any $\boldsymbol{y} \in Y$, a 1-nearest-neighbor regressor $\hat{\boldsymbol{\phi}}$ leads to $\|\hat{\boldsymbol{\phi}}(\boldsymbol{y}) - \boldsymbol{\phi}(\boldsymbol{y})\|_2 \le \epsilon$.*

Lemma 3.2 (Lower bound of sample complexity for ϵ/L-cover). *To achieve ϵ/L-cover of Y, the size of the training set $N \ge N_0(\epsilon) := \frac{\mathrm{vol}(Y)}{\mathrm{vol}_0}\left(\frac{L}{\epsilon}\right)^d$, where vol_0 is the volume of unit ball in d-dimension.*

Please find all proofs in the Appendix. While we do not rule out a more advanced regressor than 1-nearest-neighbor that leads to better sample complexity, the lemmas demonstrate that the Lipschitz constant L plays an important role in sample complexity.

3.4.2 Difference between Cost and Solution Regression

In the following we will show that in certain cases, the direct prediction $\boldsymbol{y} \mapsto \boldsymbol{x}^*(\boldsymbol{y})$ could have an infinitely large Lipschitz constant L.

To show this, let us consider a general mapping $\boldsymbol{\phi} : \mathbb{R}^d \supseteq Y \mapsto \mathbb{R}^m$. Let $\boldsymbol{\phi}(Y)$ be the image of Y under mapping $\boldsymbol{\phi}$ and $\kappa(Y)$ be the number of connected components for region Y.

Theorem 3.1 (A case of infinite Lipschitz constant). *If the minimal distance $d_{\min}$ for different connected components of $\boldsymbol{\phi}(Y)$ is strictly positive, and $\kappa(\boldsymbol{\phi}(Y)) > \kappa(Y)$, then the Lipschitz constant of the mapping $\boldsymbol{\phi}$ is infinite.*

Note that this theorem applies to a wide variety of combinatorial optimization problems. For example, when Y is a connected region and the optimization problem can be formulated as an integer program, the optimal solution set $\boldsymbol{x}^*(Y) := \{\boldsymbol{x}^*(\boldsymbol{y}) : \boldsymbol{y} \in Y\}$ is a discrete set of integral vertices, so the theorem applies. Combined with analysis in Sec. 3.4.1, we know the mapping $\boldsymbol{y} \mapsto \boldsymbol{x}^*(\boldsymbol{y})$ is hard to learn even with a lot of samples.

On the other hand, the mapping $\boldsymbol{y} \mapsto \boldsymbol{c}(\boldsymbol{y})$ can avoid too many connected components in its image $\boldsymbol{c}(Y)$, by connecting disjoint components of $\boldsymbol{x}^*(Y)$ together.

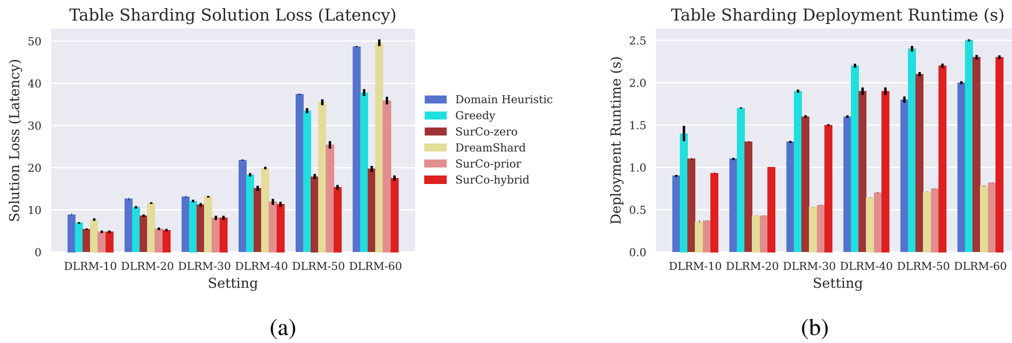


Figure 2: Table placement plan latency **(a)** and solver runtime **(b)**. We evaluate SurCo against Dreamshard (Zha et al., 2022b) a SoTA offline RL sharding tool, a domain-heuristic of assigning tables based on dimension, and a greedy heuristic based on the estimated runtime increase. Striped approaches require pre-training.

4 Empirical Evaluation

We evaluate the two variants of SurCo on two real-world settings, embedding table sharding and inverse photonic design. Both have industrial application. Each setting consists of a family of problem instances with varying feasible region and nonlinear objective function.

4.1 Embedding Table Sharding

The task of sharding embedding tables arises in the deployment of large scale neural network models which operate over both sparse and dense inputs (e.g., in recommendation systems (Zha et al., 2022a;b; Sethi et al., 2022)). Given T embedding tables and D homogeneous devices, the goal is to distribute the tables among the devices such that no device's memory limit is exceeded, while the tables are processed efficiently. Formally, let $x_{t,d}$ be the binary variable indicating whether table t is assigned to device d, and $\boldsymbol{x} := \{x_{t,d}\} \in \{0,1\}^{TD}$ be the collection of the variables. The optimization problem is:

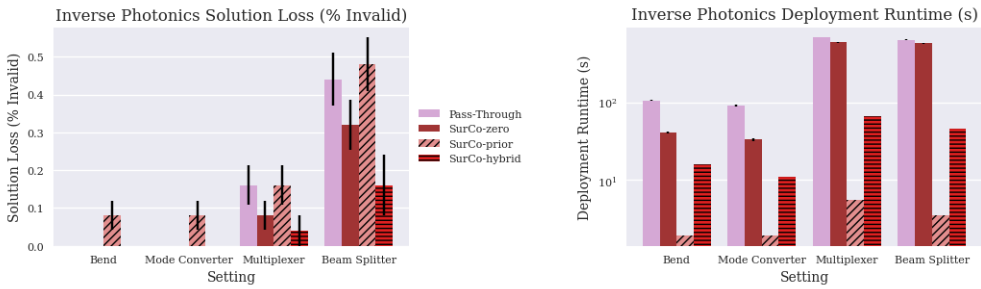
$$\min_{\boldsymbol{x}} f(\boldsymbol{x};\boldsymbol{y}) \quad \text{s.t.} \quad \boldsymbol{x} \in \Omega(\boldsymbol{y}) := \left\{ \boldsymbol{x} : \quad \forall t, \sum_t x_{t,d} = 1, \quad \forall d, \sum_t m_t x_{t,d} \le M \right\} \tag{6}$$

Here the problem description $\boldsymbol{y}$ includes table memory usage $\{m_t\}$, and capacity M of each device. $\sum_d x_{t,d} = 1$ means each table t should be assigned to exactly one device, and $\sum_t m_t x_{t,d} \le M$ means the memory consumption at each device d should not exceed its capacity. The nonlinear cost function $f(\boldsymbol{x};\boldsymbol{y})$ is the *latency*, i.e., the runtime of the longest-running device. Due to shared computation (e.g., batching) among the group of assigned tables, and communication costs across devices, the objective is highly nonlinear. $f(\boldsymbol{x};\boldsymbol{y})$ is well-approximated by a sharding plan runtime estimator proposed by Dreamshard (Zha et al., 2022b).

SurCo learns to predict $T \times D$ surrogate cost $\hat{c}_{t,d}$, one for each potential table-device assignment. During training, the gradients through combinatorial solver $\partial \boldsymbol{g}/\partial \boldsymbol{c}$ are computed via CVXPYLayers (Agrawal et al., 2019a) and the integrality constraints are relaxed. We found that in practice, we obtained solutions that were mostly integral in that only one table on any given device was fractional. At test time we solve for the integer solution using SCIP (Achterberg, 2009).

Settings. We evaluate SurCo on the publicly available Deep Learning Recommendation Model (DLRM) dataset (Naumov et al., 2019). We consider 6 settings: 10, 20, 30, 40, 50, and 60 tables are placed to 4 devices with each GPU device having a 5GB memory limit. Each setting has 100 problem instances (50 training and 50 test).

Baselines. For SurCo-zero baselines, we use Greedy that greedily allocates tables to devices while observing memory limits according to the predicted latency f, and Domain-Heuristic, the domain-expert algorithm of allocating tables to balance the aggregate dimension (Zha et al., 2022b). For SurCo-prior, we use Dreamshard, the SoTA embedding table sharding algorithm that requires training an offline RL policy.



(a) (b)

Figure 3: **(a)** The solution loss (% of failed instances when the design loss is not 0), and **(b)** test time solver runtime in log scale. For both, lower is better. We compare against the pass-through gradient approach proposed in Schubert et al. (2022). We observe that `SurCo-prior` achieves similar success rates to the previous approach `Pass-through` with a substantially improved runtime. Additionally, `SurCo-zero` runs comparably or faster, while finding more valid solutions than `Pass-through`. `SurCo-hybrid` obtains valid solutions most often and is faster than `SurCo-zero` at the expense of pretraining. Striped approaches use pretraining.

Results. Fig. 2, `SurCo-zero` finds lower latency sharding plans than the baselines, while it takes slightly longer than `Domain-Heuristic` and DreamShard due to taking optimization steps rather than selecting based on a heuristic feature or reinforcement learned policy. `SurCo-prior` obtains lower latency solutions in about the same time as DreamShard with a slight increase in overhead due to using SCIP (Achterberg, 2009), a branch and bound MILP solver. Lastly, `SurCo-hybrid` obtains the best solutions in terms of solution quality and has runtime comparable to `SurCo-zero` since at test time it performs similar operations. In smaller problem instances ($T = 10$ to $T = 40$), `SurCo-prior` obtains better quality solutions than its impromptu counterpart, `SurCo-zero`, likely due to training on a variety of examples and being able to better escape local optima in any given problem instance as might be the case with the impromptu solver. However, as the problem size increases and more tables are available for placement, `SurCo-zero` gives better performance by optimizing for the test instances in question as opposed to `SurCo-prior` which only uses training data to obtain surrogate costs. Using `SurCo-hybrid`, we are able to obtain the best quality solutions but incur the upfront cost of pretraining and the deployment-time cost of optimizing the coefficients on-the-fly.

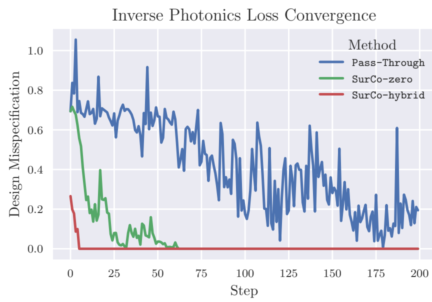
4.2 Inverse Photonic Design

Photonic devices play an important role in high-speed communication (Marpaung et al., 2019), quantum computing (Arrazola et al., 2021), and machine learning hardware acceleration (Wetzstein et al., 2020). The photonic components can be formulated as a binary 2D grid, with each cell being filled or void. There are constraints for binary patterns: only those that can be drawn by a physical brush instrument with certain cross shape can be manufactured.

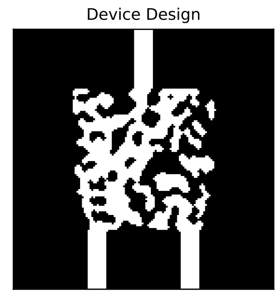
It remains challenging to find designs that are both manufacturable and satisfy design specifications (e.g., beam bending, wavelength-sensitive beam splitting). An example solution developed by `SurCo` is shown in Figures 4b and 4c: coming from the top, beams are routed to bottom left or right, depending on their wavelength. The solution is also manufacturable: a 3-by-3 brush cross can fit in all filled and void space.

Given the design, existing work (Hughes et al., 2019) enables differentiation of the design misspecification cost, evaluated as how far off the transmission of the wavelengths of interest is from the desired locations, with zero design loss meaning that the specification is satisfied. Researchers also develop a standard benchmark of inverse photonic design problems (Schubert et al., 2022).

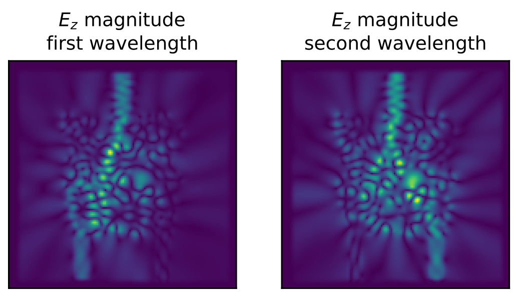
Settings. We train and evaluate our approaches and compare against the "Pass-Through" method (Schubert et al., 2022) on randomly generated instances of the four types of problems in Schubert et al. (2022): Waveguide Bend, Mode Converter, Wavelengths Division Multiplexer, and Beam Splitter. We generate 50 instances in each setting (25 training/25 test). Further generation details are in the appendix. We evaluated several nonlinear optimization algorithms described in the ap-



(a) Loss Convergence



(b) Device



(c) Wave Mangitude

Figure 4: Inverse photonic design convergence for a ceviche challenge instance (Schubert et al., 2022). `SurCo-zero` smoothly lowers the loss while the pass-through baseline yields noisier convergence. Also, `SurCo-hybrid` starts out with a high-quality solution and fine-tunes until an optimal solution is reached. We also visualize the `SurCo-zero` solution with magnitudes of the two wavelengths of interest which we successfully route from the input at the top to the two different waveguides at the bottom.

pendix, such as genetic algorithms and derivative-free optimization, which failed to find physically feasible solutions. In each setting we consider two wavelengths (1270nm/1290nm), and optimize at a resolution of 40nm. We visualize the results on test instances in Fig. 3.

Results. Fig. 3, `SurCo-zero` consistently finds as many or more valid photonic devices compared to the `Pass-Through` baseline (Schubert et al., 2022). Additionally, since the on-the-fly solvers stop when they either find a valid solution, or reach a maximum of 200 steps, the runtime of `SurCo-zero` is slightly lower than the `Pass-Through` baseline. `SurCo-prior` obtains similar success rates as the `Pass-Through` baseline while taking two orders of magnitude less time as it does not require expensive impromptu optimization or multiple evaluations of the nonlinear objective, making `SurCo-prior` a promising approach for large-scale settings or when solving many slightly-varied instances. Lastly, `SurCo-hybrid` performs best in terms of solution loss, finding valid solutions more often than the other approaches. It also takes less runtime than the other on-the-fly approaches since it is able to reach valid solutions faster, although it still requires optimization on-the-fly so it takes longer than `SurCo-prior`.

We visualize the convergence of impromptu solvers in Fig. 4a where `SurCo-zero` has smoother and faster convergence compared to the `Pass-through` approach. Here, aligned gradients from a differentiable solver rather than pass-through gradients enables `SurCo-zero` to modify the surrogate coefficients to improve the design loss.

5 Related Work

Differentiable Optimization Previous work differentiated through several optimization problems, calculating how changes in input parameters impact the optimal solution. Initially, a differentiable convex quadratic programming solver called OptNet (Amos & Kolter, 2017) proposed to implicitly differentiate the optimal solution with respect to input parameters through the KKT optimality conditions, a set of linear equations that determined the optimal solution. Following this, researchers differentiated through linear programs (Wilder et al., 2019a), submodular optimization problems (Djolonga & Krause, 2017; Wilder et al., 2019a), cone programs (Agrawal et al., 2019a;b), MaxSAT (Wang et al., 2019), Mixed Integer Linear Programming (Ferber et al., 2020; Mandi et al., 2020), Integer Linear Programming (Mandi et al., 2020), dynamic programming solvers Demirovic et al. (2020), blackbox discrete linear optimizers (Pogančić et al., 2019; Rolínek et al., 2020a;b), maximum likelihood estimation (Niepert et al., 2021), kmeans clustering (Wilder et al., 2019b), knapsack (Guler et al., 2022; Demirović et al., 2019), the cross-entropy method (Amos & Yarats, 2020), and SVM training (Lee et al., 2019). Additionally, Wang et al. (2020a) learned to linearly combine LP variables. `SurCo` can use these differentiable surrogates based on the problem domain.

Task Based Learning Researchers have investigated task-based learning, where we are given a distribution of linear or quadratic optimization problems and asked to train an optimizer with the true linear or quadratic objective hidden at test time but available for training (Elmachtoub & Grigas, 2022; Donti et al., 2017). There are several theoretically motivated approaches in this space (El Balghiti et al., 2019; Liu & Grigas, 2021; Hu et al., 2022); however, they assume access to ground truth linear or quadratic coefficients at train time but not at test time, unlike our considered nonlinear nonconvex combinatorial settings. Donti et al. (2021) predicts solutions for continuous optimization problems with nonlinear constraints. The approach relies on the continuous feasible region to predict and correct initial solutions in a differentiable manner, something not trivially applicable to the combinatorial setting. Machine learning is also used to guide combinatorial algorithms. Several approaches produce solutions to combinatorial problems (Zhang & Dietterich, 1995; Khalil et al., 2017; Kool et al., 2018; Nazari et al., 2018; Zha et al., 2022a;b). Here, the approaches are limited to searching simple feasible regions by iteratively building solutions for problems like routing, assignment, or covering. Other approaches set parameters that improve the runtime of exact solvers (Khalil et al., 2016; Bengio et al., 2021). However, these approaches are unable to handle more complex combinatorial constraints that arise in practice such as those in inverse photonic design.

Learning Latent Space for Optimization As we learn latent linear objectives to optimize nonlinear functions, other approaches learn latent embeddings for faster solving. Faloutsos & Lin (1995) proposed FastMap, which learns latent object embeddings for efficient search. Variants of FastMap are used in graph optimization and shortest path (Cohen et al., 2018; Hu et al., 2022; Li et al., 2019). Wang et al. (2020b; 2021a); Yang et al. (2021); Zhao et al. (2022) use monte carlo tree search to perform single and multi-objective blackbox optimization by learning to split the search space.

Mixed Integer Nonlinear Programming (MINLP) `SurCo-zero` falls into the broad family of MINLP solvers, and specifically we are addressing problems optimizing nonlinear and nonconvex objectives over discrete feasible regions with linear constraints. Specialized solvers handle many problem variants in the MINLP space (Burer & Letchford, 2012; Belotti et al., 2013); however, scalabliliy in the nonconvex setting is usually obtained by optimization experts who rely on problem-specific solving techniques such as making piecewise linear approximations, convexifying the objective, or exploiting special structure.

6 CONCLUSION

We introduced `SurCo`, a method for learning linear surrogates for combinatorial nonlinear optimization problems. `SurCo` learns linear objective coefficients for a surrogate solver which results in solutions that minimize the nonlinear loss via gradient descent. At its core, `SurCo` differentiates through the surrogate solver which maps the predicted coefficients to a combinatorially feasible solution, combining the flexibility of gradient-based optimization with the structure of combinatorial solvers. We presented three variants of `SurCo`, `SurCo-zero` which optimizes individual instances, `SurCo-prior` which trains a coefficient prediction model offline, and `SurCo-hybrid` which fine-tunes the coefficients predicted by `SurCo-prior` on individual test instances. We evaluated these approaches on two domains against the state of the art approaches used in industry, obtaining better solution quality for similar or better runtime in the embedding table sharding domain, and quickly identifying viable photonic devices.

REFERENCES

Tobias Achterberg. Scip: solving constraint integer programs. *Mathematical Programming Computation*, 1(1):1–41, 2009.

Akshay Agrawal, Brandon Amos, Shane Barratt, Stephen Boyd, Steven Diamond, and J Zico Kolter. Differentiable convex optimization layers. *Advances in neural information processing systems*, 32, 2019a.

Akshay Agrawal, Shane Barratt, Stephen Boyd, Enzo Busseti, and Walaa M Moursi. Differentiating through a cone program. *J. Appl. Numer. Optim*, 1(2):107–115, 2019b.

Brandon Amos and J Zico Kolter. Optnet: Differentiable optimization as a layer in neural networks. In *International Conference on Machine Learning*, pp. 136–145. PMLR, 2017.

Brandon Amos and Denis Yarats. The differentiable cross-entropy method. In *International Conference on Machine Learning*, pp. 291–302. PMLR, 2020.

Juan M Arrazola, Ville Bergholm, Kamil Brádler, Thomas R Bromley, Matt J Collins, Ish Dhand, Alberto Fumagalli, Thomas Gerrits, Andrey Goussev, Lukas G Helt, et al. Quantum circuits with many photons on a programmable nanophotonic chip. *Nature*, 591(7848):54–60, 2021.

Gah-Yi Ban and Cynthia Rudin. The big data newsvendor: Practical insights from machine learning. *Operations Research*, 67(1):90–108, 2019.

Pietro Belotti, Christian Kirches, Sven Leyffer, Jeff Linderoth, James Luedtke, and Ashutosh Mahajan. Mixed-integer nonlinear optimization. *Acta Numerica*, 22:1–131, 2013.

Yoshua Bengio, Andrea Lodi, and Antoine Prouvost. Machine learning for combinatorial optimization: a methodological tour d'horizon. *European Journal of Operational Research*, 290(2): 405–421, 2021.

Quentin Berthet, Mathieu Blondel, Olivier Teboul, Marco Cuturi, Jean-Philippe Vert, and Francis Bach. Learning with differentiable pertubed optimizers. *Advances in neural information processing systems*, 33:9508–9519, 2020.

James Bradbury, Roy Frostig, Peter Hawkins, Matthew James Johnson, Chris Leary, Dougal Maclaurin, George Necula, Adam Paszke, Jake VanderPlas, Skye Wanderman-Milne, and Qiao Zhang. JAX: composable transformations of Python+NumPy programs, 2018. URL `http://github.com/google/jax`.

Samuel Burer and Adam N Letchford. Non-convex mixed-integer nonlinear programming: A survey. *Surveys in Operations Research and Management Science*, 17(2):97–106, 2012.

Vasek Chvatal, Vaclav Chvatal, et al. *Linear programming*. Macmillan, 1983.

Liron Cohen, Tansel Uras, Shiva Jahangiri, Aliyah Arunasalam, Sven Koenig, and TK Satish Kumar. The fastmap algorithm for shortest path computations. In *IJCAI*, 2018.

Alison Cozad, Nikolaos V Sahinidis, and David C Miller. Learning surrogate models for simulation-based optimization. *AIChE Journal*, 60(6):2211–2227, 2014.

Emir Demirović, Peter J Stuckey, James Bailey, Jeffrey Chan, Christopher Leckie, Kotagiri Ramamohanarao, and Tias Guns. Predict+ optimise with ranking objectives: Exhaustively learning linear functions. In *Proceedings of the Twenty-Eighth International Joint Conference on Artificial Intelligence, IJCAI 2019, Macao, China, August 10-16, 2019*, pp. 1078–1085. International Joint Conferences on Artificial Intelligence, 2019.

Emir Demirovic, Peter J Stuckey, Tias Guns, James Bailey, Christopher Leckie, Kotagiri Ramamohanarao, and Jeffrey Chan. Dynamic programming for predict+ optimise. In *The Thirty-Fourth AAAI Conference on Artificial Intelligence, AAAI 2020, The Thirty-Second Innovative Applications of Artificial Intelligence Conference, IAAI 2020, The Tenth AAAI Symposium on Educational Advances in Artificial Intelligence, EAAI 2020, New York, NY, USA, February 7-12, 2020*, pp. 1444–1451. AAAI Press, 2020.

Josip Djolonga and Andreas Krause. Differentiable learning of submodular models. *Advances in Neural Information Processing Systems*, 30, 2017.

Priya Donti, Brandon Amos, and J Zico Kolter. Task-based end-to-end model learning in stochastic optimization. *Advances in neural information processing systems*, 30, 2017.

Priya L. Donti, David Rolnick, and J Zico Kolter. DC3: A learning method for optimization with hard constraints. In *International Conference on Learning Representations*, 2021. URL https://openreview.net/forum?id=V1ZHVxJ6dSS.

Othman El Balghiti, Adam N Elmachtoub, Paul Grigas, and Ambuj Tewari. Generalization bounds in the predict-then-optimize framework. *Advances in neural information processing systems*, 32, 2019.

Adam N Elmachtoub and Paul Grigas. Smart "predict, then optimize". *Management Science*, 68(1): 9–26, 2022.

Christos Faloutsos and King-Ip Lin. Fastmap: A fast algorithm for indexing, data-mining and visualization of traditional and multimedia datasets. In *Proceedings of the 1995 ACM SIGMOD International Conference on Management of Data*, SIGMOD '95, pp. 163–174, New York, NY, USA, 1995. Association for Computing Machinery. ISBN 0897917316. doi: 10.1145/223784.223812. URL https://doi.org/10.1145/223784.223812.

Aaron Ferber, Bryan Wilder, Bistra Dilkina, and Milind Tambe. Mipaal: Mixed integer program as a layer. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 34, pp. 1504–1511, 2020.

Ahmed Fawzy Gad. Pygad: An intuitive genetic algorithm python library, 2021.

Abhijit Gosavi et al. *Simulation-based optimization*. Springer, 2015.

Ali Ugur Guler, Emir Demirović, Jeffrey Chan, James Bailey, Christopher Leckie, and Peter J Stuckey. A divide and conquer algorithm for predict+ optimize with non-convex problems. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 36, pp. 3749–3757, 2022.

Gurobi Optimization, LLC. Gurobi Optimizer Reference Manual, 2022. URL https://www.gurobi.com.

Yichun Hu, Nathan Kallus, and Xiaojie Mao. Fast rates for contextual linear optimization. *Management Science*, 2022.

Tyler W Hughes, Ian AD Williamson, Momchil Minkov, and Shanhui Fan. Forward-mode differentiation of maxwell's equations. *ACS Photonics*, 6(11):3010–3016, 2019.

John Jumper, Richard Evans, Alexander Pritzel, Tim Green, Michael Figurnov, Olaf Ronneberger, Kathryn Tunyasuvunakool, Russ Bates, Augustin Žídek, Anna Potapenko, et al. Highly accurate protein structure prediction with alphafold. *Nature*, 596(7873):583–589, 2021.

Elias Khalil, Pierre Le Bodic, Le Song, George Nemhauser, and Bistra Dilkina. Learning to branch in mixed integer programming. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 30, 2016.

Elias Khalil, Hanjun Dai, Yuyu Zhang, Bistra Dilkina, and Le Song. Learning combinatorial optimization algorithms over graphs. *Advances in neural information processing systems*, 30, 2017.

Wouter Kool, Herke van Hoof, and Max Welling. Attention, learn to solve routing problems! In *International Conference on Learning Representations*, 2018.

Bernhard Korte and Dirk Hausmann. An analysis of the greedy heuristic for independence systems. In *Annals of Discrete Mathematics*, volume 2, pp. 65–74. Elsevier, 1978.

Slawomir Koziel, Nurullah Çalık, Peyman Mahouti, and Mehmet A Belen. Accurate modeling of antenna structures by means of domain confinement and pyramidal deep neural networks. *IEEE Transactions on Antennas and Propagation*, 70(3):2174–2188, 2021.

Ailsa H Land and Alison G Doig. An automatic method for solving discrete programming problems. In *50 Years of Integer Programming 1958-2008*, pp. 105–132. Springer, 2010.

Kwonjoon Lee, Subhransu Maji, Avinash Ravichandran, and Stefano Soatto. Meta-learning with differentiable convex optimization. In *Proceedings of the IEEE/CVF conference on computer vision and pattern recognition*, pp. 10657–10665, 2019.

Jiaoyang Li, Ariel Felner, Sven Koenig, and TK Satish Kumar. Using fastmap to solve graph problems in a euclidean space. In *Proceedings of the international conference on automated planning and scheduling*, volume 29, pp. 273–278, 2019.

Sirui Li, Zhongxia Yan, and Cathy Wu. Learning to delegate for large-scale vehicle routing. *Advances in Neural Information Processing Systems*, 34:26198–26211, 2021.

Zhuwen Li, Qifeng Chen, and Vladlen Koltun. Combinatorial optimization with graph convolutional networks and guided tree search. *Advances in neural information processing systems*, 31, 2018.

Heyuan Liu and Paul Grigas. Risk bounds and calibration for a smart predict-then-optimize method. *Advances in Neural Information Processing Systems*, 34:22083–22094, 2021.

Giampaolo Liuzzi, Stefano Lucidi, and Francesco Rinaldi. Derivative-free methods for mixed-integer constrained optimization problems. *Journal of Optimization Theory and Applications*, 164(3):933–965, 2015.

Jayanta Mandi, Peter J Stuckey, Tias Guns, et al. Smart predict-and-optimize for hard combinatorial optimization problems. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 34, pp. 1603–1610, 2020.

David Marpaung, Jianping Yao, and José Capmany. Integrated microwave photonics. *Nature photonics*, 13(2):80–90, 2019.

Nina Mazyavkina, Sergey Sviridov, Sergei Ivanov, and Evgeny Burnaev. Reinforcement learning for combinatorial optimization: A survey. *Computers & Operations Research*, 134:105400, 2021.

Azalia Mirhoseini, Anna Goldie, Mustafa Yazgan, Joe Wenjie Jiang, Ebrahim Songhori, Shen Wang, Young-Joon Lee, Eric Johnson, Omkar Pathak, Azade Nazi, et al. A graph placement methodology for fast chip design. *Nature*, 594(7862):207–212, 2021.

Ryo Nagai, Ryosuke Akashi, and Osamu Sugino. Completing density functional theory by machine learning hidden messages from molecules. *npj Computational Materials*, 6(1):1–8, 2020.

Maxim Naumov, Dheevatsa Mudigere, Hao-Jun Michael Shi, Jianyu Huang, Narayanan Sundaraman, Jongsoo Park, Xiaodong Wang, Udit Gupta, Carole-Jean Wu, Alisson G. Azzolini, Dmytro Dzhulgakov, Andrey Mallevich, Ilia Cherniavskii, Yinghai Lu, Raghuraman Krishnamoorthi, Ansha Yu, Volodymyr Kondratenko, Stephanie Pereira, Xianjie Chen, Wenlin Chen, Vijay Rao, Bill Jia, Liang Xiong, and Misha Smelyanskiy. Deep learning recommendation model for personalization and recommendation systems. *CoRR*, abs/1906.00091, 2019. URL https://arxiv.org/abs/1906.00091.

Mohammadreza Nazari, Afshin Oroojlooy, Lawrence Snyder, and Martin Takác. Reinforcement learning for solving the vehicle routing problem. *Advances in neural information processing systems*, 31, 2018.

Mathias Niepert, Pasquale Minervini, and Luca Franceschi. Implicit mle: backpropagating through discrete exponential family distributions. *Advances in Neural Information Processing Systems*, 34:14567–14579, 2021.

Adam Paszke, Sam Gross, Francisco Massa, Adam Lerer, James Bradbury, Gregory Chanan, Trevor Killeen, Zeming Lin, Natalia Gimelshein, Luca Antiga, Alban Desmaison, Andreas Kopf, Edward Yang, Zachary DeVito, Martin Raison, Alykhan Tejani, Sasank Chilamkurthy, Benoit Steiner, Lu Fang, Junjie Bai, and Soumith Chintala. Pytorch: An imperative style, high-performance deep learning library. In H. Wallach, H. Larochelle, A. Beygelzimer, F. d'Alché-Buc, E. Fox, and R. Garnett (eds.), *Advances in Neural Information Processing Systems 32*, pp.

8024–8035. Curran Associates, Inc., 2019. URL http://papers.neurips.cc/paper/9015-pytorch-an-imperative-style-high-performance-deep-learning-library.pdf.

Marin Vlastelica Pogančić, Anselm Paulus, Vit Musil, Georg Martius, and Michal Rolinek. Differentiation of blackbox combinatorial solvers. In *International Conference on Learning Representations*, 2019.

J. Rapin and O. Teytaud. Nevergrad - A gradient-free optimization platform. https://GitHub.com/FacebookResearch/Nevergrad, 2018.

Edward M Reingold and Robert E Tarjan. On a greedy heuristic for complete matching. *SIAM Journal on Computing*, 10(4):676–681, 1981.

Michal Rolínek, Vít Musil, Anselm Paulus, Marin Vlastelica, Claudio Michaelis, and Georg Martius. Optimizing rank-based metrics with blackbox differentiation. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp. 7620–7630, 2020a.

Michal Rolínek, Paul Swoboda, Dominik Zietlow, Anselm Paulus, Vít Musil, and Georg Martius. Deep graph matching via blackbox differentiation of combinatorial solvers. In *European Conference on Computer Vision*, pp. 407–424. Springer, 2020b.

Sebastian Ruder. An overview of gradient descent optimization algorithms. *arXiv preprint arXiv:1609.04747*, 2016.

Martin F. Schubert, Alfred K. C. Cheung, Ian A. D. Williamson, Aleksandra Spyra, and David H. Alexander. Inverse design of photonic devices with strict foundry fabrication constraints. *ACS Photonics*, 9(7):2327–2336, 2022. doi: 10.1021/acsphotonics.2c00313.

Geet Sethi, Bilge Acun, Niket Agarwal, Christos Kozyrakis, Caroline Trippel, and Carole-Jean Wu. Recshard: statistical feature-based memory optimization for industry-scale neural recommendation. In *Proceedings of the 27th ACM International Conference on Architectural Support for Programming Languages and Operating Systems*, pp. 344–358, 2022.

Dan Simon. *Evolutionary optimization algorithms*. John Wiley & Sons, 2013.

Benoit Steiner, Chris Cummins, Horace He, and Hugh Leather. Value learning for throughput optimization of deep learning workloads. In A. Smola, A. Dimakis, and I. Stoica (eds.), *Proceedings of Machine Learning and Systems*, volume 3, pp. 323–334, 2021. URL https://proceedings.mlsys.org/paper/2021/file/73278a4a86960eeb576a8fd4c9ec6997-Paper.pdf.

Guido Van Rossum and Fred L. Drake. *Python 3 Reference Manual*. CreateSpace, Scotts Valley, CA, 2009. ISBN 1441412697.

Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Łukasz Kaiser, and Illia Polosukhin. Attention is all you need. *Advances in neural information processing systems*, 30, 2017.

Stefan Voß, Silvano Martello, Ibrahim H Osman, and Catherine Roucairol. *Meta-heuristics: Advances and trends in local search paradigms for optimization*. Springer Science & Business Media, 2012.

Kai Wang, Bryan Wilder, Andrew Perrault, and Milind Tambe. Automatically learning compact quality-aware surrogates for optimization problems. *Advances in Neural Information Processing Systems*, 33:9586–9596, 2020a.

Linnan Wang, Rodrigo Fonseca, and Yuandong Tian. Learning search space partition for black-box optimization using monte carlo tree search. *Advances in Neural Information Processing Systems*, 33:19511–19522, 2020b.

Linnan Wang, Saining Xie, Teng Li, Rodrigo Fonseca, and Yuandong Tian. Sample-efficient neural architecture search by learning actions for monte carlo tree search. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 2021a.

Po-Wei Wang, Priya Donti, Bryan Wilder, and Zico Kolter. Satnet: Bridging deep learning and logical reasoning using a differentiable satisfiability solver. In *International Conference on Machine Learning*, pp. 6545–6554. PMLR, 2019.

Xiaodi Wang, Youbo Liu, Junbo Zhao, Chang Liu, Junyong Liu, and Jinyue Yan. Surrogate model enabled deep reinforcement learning for hybrid energy community operation. *Applied Energy*, 289:116722, 2021b.

Gordon Wetzstein, Aydogan Ozcan, Sylvain Gigan, Shanhui Fan, Dirk Englund, Marin Soljačić, Cornelia Denz, David AB Miller, and Demetri Psaltis. Inference in artificial intelligence with deep optics and photonics. *Nature*, 588(7836):39–47, 2020.

Bryan Wilder, Bistra Dilkina, and Milind Tambe. Melding the data-decisions pipeline: Decision-focused learning for combinatorial optimization. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 33, pp. 1658–1665, 2019a.

Bryan Wilder, Eric Ewing, Bistra Dilkina, and Milind Tambe. End to end learning and optimization on graphs. *Advances in Neural Information Processing Systems*, 32, 2019b.

Laurence A Wolsey. An analysis of the greedy algorithm for the submodular set covering problem. *Combinatorica*, 2(4):385–393, 1982.

Laurence A Wolsey. Mixed integer programming. *Wiley Encyclopedia of Computer Science and Engineering*, pp. 1–10, 2007.

Kevin Yang, Tianjun Zhang, Chris Cummins, Brandon Cui, Benoit Steiner, Linnan Wang, Joseph E Gonzalez, Dan Klein, and Yuandong Tian. Learning space partitions for path planning. *Advances in Neural Information Processing Systems*, 34:378–391, 2021.

Yingjun Ye, Xiaohui Zhang, and Jian Sun. Automated vehicle's behavior decision making using deep reinforcement learning and high-fidelity simulation environment. *Transportation Research Part C: Emerging Technologies*, 107:155–170, 2019.

Daochen Zha, Louis Feng, Bhargav Bhushanam, Dhruv Choudhary, Jade Nie, Yuandong Tian, Jay Chae, Yinbin Ma, Arun Kejariwal, and Xia Hu. Autoshard: Automated embedding table sharding for recommender systems. In *Proceedings of the 28th ACM SIGKDD Conference on Knowledge Discovery and Data Mining*, pp. 4461–4471, 2022a.

Daochen Zha, Louis Feng, Qiaoyu Tan, Zirui Liu, Kwei-Herng Lai, Bhushanam Bhargav, Yuandong Tian, Arun Kejariwal, and Xia Hu. Dreamshard: Generalizable embedding table placement for recommender systems. In *Advances in Neural Information Processing Systems*, 2022b.

Wei Zhang and Thomas G Dietterich. A reinforcement learning approach to job-shop scheduling. In *IJCAI*, volume 95, pp. 1114–1120. Citeseer, 1995.

Yiyang Zhao, Linnan Wang, Kevin Yang, Tianjun Zhang, Tian Guo, and Yuandong Tian. Multi-objective optimization by learning space partition. In *International Conference on Learning Representations*, 2022. URL `https://openreview.net/forum?id=FlwzVjfMryn`.

Yanqi Zhou, Sudip Roy, Amirali Abdolrashidi, Daniel Wong, Peter Ma, Qiumin Xu, Hanxiao Liu, Phitchaya Phothilimtha, Shen Wang, Anna Goldie, et al. Transferable graph optimizers for ml compilers. *Advances in Neural Information Processing Systems*, 33:13844–13855, 2020.

A PROOFS

Lemma 3.1 (Sufficient condition of prediction with ϵ-accuracy). *If the dataset $\mathcal{D}_{\text{direct}}$ (ϵ/L)-cover Y, then for any $\boldsymbol{y} \in Y$, a 1-nearest-neighbor regressor $\hat{\boldsymbol{\phi}}$ leads to $\|\hat{\boldsymbol{\phi}}(\boldsymbol{y}) - \boldsymbol{\phi}(\boldsymbol{y})\|_2 \leq \epsilon$.*

Proof. Since the dataset is a ϵ/L-cover, for any $\boldsymbol{y} \in Y$, there exists at least one $\boldsymbol{y}_i$ so that $\|\boldsymbol{y} - \boldsymbol{y}_i\|_2 \leq \epsilon/L$. Let $\boldsymbol{y}_{\text{nn}}$ be the nearest neighbor of $\boldsymbol{y}$, and we have:

$$\|\boldsymbol{y} - \boldsymbol{y}_{\text{nn}}\|_2 \leq \|\boldsymbol{y} - \boldsymbol{y}_i\|_2 \leq \epsilon/L \tag{7}$$

From the Lipschitz condition and the definition of 1-nearest-neighbor classifier ($\hat{\boldsymbol{\phi}}(\boldsymbol{y}) = \boldsymbol{\phi}(\boldsymbol{y}_{\text{nn}})$), we know that

$$\|\boldsymbol{\phi}(\boldsymbol{y}) - \hat{\boldsymbol{\phi}}(\boldsymbol{y})\|_2 = \|\boldsymbol{\phi}(\boldsymbol{y}) - \boldsymbol{\phi}(\boldsymbol{y}_{\text{nn}})\|_2 \leq L\|\boldsymbol{y} - \boldsymbol{y}_{\text{nn}}\|_2 \leq \epsilon \tag{8}$$

□

Lemma 3.2 (Lower bound of sample complexity for ϵ/L-cover). *To achieve ϵ/L-cover of Y, the size of the training set $N \geq N_0(\epsilon) := \frac{\text{vol}(Y)}{\text{vol}_0}\left(\frac{L}{\epsilon}\right)^d$, where vol_0 is the volume of unit ball in d-dimension.*

Proof. We prove by contradiction. If $N < N_0(\epsilon)$, then for each training sample $(\boldsymbol{y}_i, \boldsymbol{\phi}_i)$, we create a ball $B_i := B(\boldsymbol{y}_i, \epsilon/L)$. Since

$$\text{vol}\left(\bigcup_{i=1}^N B_i \cap Y\right) \leq \text{vol}\left(\bigcup_{i=1}^N B_i\right) \leq \sum_{i=1}^N \text{vol}(B_i) = N\text{vol}_0\left(\frac{\epsilon}{L}\right)^d < \text{vol}(Y) \tag{9}$$

Therefore, there exists at least one $\boldsymbol{y} \in Y$ so that $\boldsymbol{y} \notin B_i$ for any $1 \leq i \leq N$. This means that $\boldsymbol{y}$ is not ϵ/L-covered. □

Theorem 3.1 (A case of infinite Lipschitz constant). *If the minimal distance $d_{\min}$ for different connected components of $\boldsymbol{\phi}(Y)$ is strictly positive, and $\kappa(\boldsymbol{\phi}(Y)) > \kappa(Y)$, then the Lipschitz constant of the mapping $\boldsymbol{\phi}$ is infinite.*

Proof. Let $R_1, R_2, \ldots, R_K$ be the $K = \kappa(\boldsymbol{\phi}(Y))$ connected components of $\boldsymbol{\phi}(Y)$, and $Y_1, Y_2, \ldots, Y_J$ be the $J = \kappa(Y)$ connected components of Y. From the condition, we know that $\min_{k\neq k'} \text{dist}(R_k, R_{k'}) = d_{\min} > 0$.

We have $R_k \cap R_{k'} = \emptyset$ for $k \neq k'$. Each R_k has a pre-image $S_k := \boldsymbol{\phi}^{-1}(R_k) \subseteq Y$. These pre-images $\{S_k\}_{k=1}^K$ form a partition of Y since

- $S_k \cap S_{k'} = \emptyset$ for $k \neq k'$ since any $\boldsymbol{y} \in Y$ cannot be mapped to more than one connected components;
- $\bigcup_{k=1}^K S_k = \bigcup_{k=1}^K \boldsymbol{\phi}^{-1}(R_k) = \boldsymbol{\phi}^{-1}\left(\bigcup_{k=1}^K R_k\right) = \boldsymbol{\phi}^{-1}(\boldsymbol{\phi}(S)) = S$.

Since $K = \kappa(\boldsymbol{\phi}(Y)) > \kappa(Y)$, by pigeonhole principle, there exists one Y_j that contains at least part of the two pre-images S_k and $S_{k'}$ with $k \neq k'$. This means that

$$S_k \cap Y_j \neq \emptyset, \quad S_{k'} \cap Y_j \neq \emptyset \tag{10}$$

Then we pick $\boldsymbol{y} \in S_k \cap Y_j$ and $\boldsymbol{y}' \in S_{k'} \cap Y_j$. Since $\boldsymbol{y}, \boldsymbol{y}' \in Y_j$ and Y_j is a connected component, there exists a continuous path $\gamma : [0, 1] \mapsto Y_j$ so that $\gamma(0) = \boldsymbol{y}$ and $\gamma(1) = \boldsymbol{y}'$. Therefore, we have $\boldsymbol{\phi}(\gamma(0)) \in R_k$ and $\boldsymbol{\phi}(\gamma(1)) \in R_{k'}$. Let $t_0 := \sup\{t : t \in [0, 1], \boldsymbol{\phi}(\gamma(t)) \in R_k\}$, then $0 \leq t_0 < 1$. For any sufficiently small $\epsilon > 0$, we have:

- By the definition of sup, we know there exists $t_0 - \epsilon \leq t' \leq t_0$ so that $\boldsymbol{\phi}(\gamma(t')) \in R_k$.
- Picking $t'' = t_0 + \epsilon < 1$, then $\boldsymbol{\phi}(\gamma(t'')) \in R_{k''}$ with some $k'' \neq k$.

Task	Randomization
mode converter	randomize the right and left waveguide width
bend setting	randomize the waveguide width and length
beam splitter	randomize the waveguide separation, width and length
wavelength division multiplexer	randomize the input and output waveguide locations

Table 1: Task randomization of 4 different tasks in inverse photonic design.

On the other hand, by continuity of the curve γ, there exists a constant $C(t_0)$ so that $\|\gamma(t') - \gamma(t'')\|_2 \leq C(t_0)\|t' - t''\|_2 \leq 2C(t_0)\epsilon$. Then we have

$$L = \max_{\boldsymbol{y},\boldsymbol{y}' \in Y} \frac{\|\boldsymbol{\phi}(\boldsymbol{y}) - \boldsymbol{\phi}(\boldsymbol{y}')\|_2}{\|\boldsymbol{y} - \boldsymbol{y}'\|_2} \geq \frac{\|\boldsymbol{\phi}(\gamma(t')) - \boldsymbol{\phi}(\gamma(t''))\|_2}{\|\gamma(t') - \gamma(t'')\|_2} \geq \frac{d_{\min}}{2C(t_0)\epsilon} \to +\infty \tag{11}$$

□

B Experiment Details

B.1 Setups

Experiments are performed on a cluster of identical machines, each with 4 Nvidia A100 GPUs and 32 CPU cores, with 1T of RAM and 40GB of GPU memory. Additionally, we perform all operations in Python (Van Rossum & Drake, 2009) using Pytorch (Paszke et al., 2019). For embedding table placement, the nonlinear cost estimator is trained for 200 iterations and the offline-trained models of Dreamshard and `SurCo-prior` are trained against the pretrained cost estimator for 200 iterations. The DLRM Dataset Naumov et al. (2019) is available at `https://github.com/facebookresearch/dlrm_datasets`, and the dreamshard (Zha et al., 2022b) code is available at `https://github.com/daochenzha/dreamshard`. Additional details on dreamshard's model architecture and features can be obtained in the paper and codebase.

B.2 Network Architectures

B.2.1 Embedding Table Sharding

The table features are the same used in Zha et al. (2022b), and sinusoidal positional encoding Vaswani et al. (2017) is used as device features so that the learning model is able to break symmetries between the different tables and effectively group them onto homogeneous devices. The table and device features are concatenated and then fed into Dreamshard's initial fully-connected table encoding module to obtain scalar predictions $\hat{c}_{t,d}$ for each desired objective coefficient.

B.2.2 Inverse Photonic Design

Network architectures. The input design specification (a 2D image) is passed through a 3 layer convolutional neural network with ReLU activations and a final layer composed of filtering with the known brush shape. Then a tanh activation is used to obtain surrogate coefficients $\hat{\boldsymbol{c}}$, one component for each binary input variable.

This is motivated by previous work (Schubert et al., 2022) that also uses the fixed brush shape filter and tanh operation to transform the latent parameters into a continuous solution that is projected onto the space of physically feasible solutions.

Previous work formulated the projection as finding a discrete solution that minimized the dot product of the input continuous solution and proposed discrete solution. The authors then updated the continuous solution by computing gradients of the loss with respect to the discrete solution and using pass-through gradients to update the continuous solution. By comparison, our approach treats the projection as an optimization problem and updates the objective coefficients so that the resulting projected solution moves in the direction of the desired gradient.

To compute the gradient of this blackbox projection solver, we leverage the approach suggested by Pogančić et al. (2019) which calls the solver twice, once with the original coefficients, and again with coefficients that are perturbed in the direction of the incoming solution gradient as being an "improved solution". The gradient with respect to the input coefficients are then the difference between the "improved solution" and the solution for the current objective coefficients.

C Additional Failed Baselines

SOGA - Single Objective Genetic Algorithm Using PyGAD (Gad, 2021), we attempted several approaches for both table sharding and inverse photonics settings. While we were able to obtain feasible table sharding solutions, they underperformed the greedy baseline by 20%. Additionally, they were unable to find physically feasible inverse photonics solutions. We varied between random, swap, inversion, and scramble mutations and used all parent selection methods but were unable to find viable solutions.

DFL - A Derivative-Free Library We could not easily integrate DFLGEN (Liuzzi et al., 2015) into our pipelines since it operates in fortran and we needed to specify the feasible region with python in the ceviche challenges. DFLINT works in python but took more than 24 hours to run on individual instances which reached a timeout limit. We found that the much longer runtime made this inapplicable for the domains of interest.

Nevergrad We enforced integrality in Nevergrad (Rapin & Teytaud, 2018) using choice variables which selected between 0 and 1. This approach was unable to find feasible solutions for inverse photonics in less than 10 hours. For table sharding we obtained solutions by using a choice variable for each table, selecting one of the available devices. This approach was not able to outperform the greedy baseline and took longer time so it was strictly dominated by the greedy approach.