UNIFY: A Unified Policy Designing Framework for Solving Constrained Optimization Problems with Machine Learning

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ABSTRACT
The interplay between Machine Learning (ML) and Constrained Optimization (CO) has recently been the subject of increasing interest, leading to a new and prolific research area covering (e.g.) Decision Focused Learning and Constrained Reinforcement Learning. Such approaches strive to tackle complex decision problems under uncertainty over multiple stages, involving both explicit (cost function, constraints) and implicit knowledge (from data), and possibly subject to execution time restrictions. While a good degree of success has been achieved, the existing methods still have limitations in terms of both applicability and effectiveness. For problems in this class, we propose UNIFY, a unified framework to design a solution policy for complex decision-making problems. Our approach relies on a clever decomposition of the policy in two stages, namely an unconstrained ML model and a CO problem, to take advantage of the strength of each approach while compensating for its weaknesses. With a little design effort, UNIFY can generalize several existing approaches, thus extending their applicability. We demonstrate the method effectiveness on two practical problems, namely an Energy Management System and the Set Multi-cover with stochastic coverage requirements. Finally, we highlight some current challenges of our method and future research directions that can benefit from the cross-fertilization of the two fields.

1 Introduction

Methods for combining Machine Learning (ML) and Constrained Optimization (CO) for decision support have attracted considerable interest in recent years. This is motivated by the possibility to tackle complex decision making problems subject to uncertainty (sometimes over multiple stages), and having a partially specified structure where knowledge is available both in explicit form (cost function, constraints) and implicit form (historical data or simulators).

As a practical example, an Energy Management Systems (EMS) needs to allocate minimum-cost power flows from different Distributed Energy Resources (DERs) [1]. Based on actual energy prices, and forecasts on the availability of DERs and on consumption, the EMS decides which power generators should be used and whether the surplus should be stored or sold to the market. Such a problem involves hard constraints (maintaining power balance, power flow limits), a clear cost structure, elements of uncertainty that are partially known via historical data, and multiple decision stages likely subject to execution time restrictions. In this type of use case, pure CO methods struggle with robustness and scalability, while pure ML methods such as Reinforcement Learning (RL) have trouble dealing with hard constraints and combinatorial decision spaces. Motivated by the opportunity to obtain improvements via a combination of ML and CO, multiple lines of research have emerged, such as Decision Focused Learning, Constrained Reinforcement Learning, or Algorithm Configuration. While existing methods have obtained a good measure of success, to the best of the authors knowledge no existing method can deal with all the challenges we have identified.

Ideally, one wishes to obtain a solution policy capable of providing feasible (and high-quality) solutions, handling robustness, taking advantage of existing data, and with a reasonable computational load. In this paper, we argue this can

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be achieved by introducing a unification framework for a family of existing ML & CO approaches, in particular: 1) Decision Focused Learning, 2) Constrained Reinforcement Learning, 3) Algorithm Configuration and 4) Stochastic Optimization algorithms. We assume to have access to problem knowledge in the form of both a declarative formulation (namely an objective function and a set of constraints), and of historical data. The framework is then based on a two-step policy decomposition, respectively into an unconstrained ML model and a CO problem. The interface between the two components consists of a new set of “virtual” model parameters, which can serve as an additional (and potentially very useful) design handle. Since the approach is decomposition-based, multiple learning and optimization methods can be used for its implementation. In our presentation we use RL for the learning task, due to its ability to handle both non-differentiable loss functions and sequential problems. We refer to our method as UNIFY.

The paper is structured as follows: we describe two motivating use cases in section 2; in Section 3 we formalize the approach, while in Section 4 we show its relation with other hybrid and traditional methods for decision support. We present an empirical evaluation on the two use cases in Section 5 while concluding remarks are in Section 6.

2 Use Cases Description

We rely on two use cases to motivate and demonstrate our approach, i.e. an Energy Management System and a simplified production scheduling problem, for which both implicit and explicit knowledge is available in the form of:

- historical data or simulators;
- an objective function;
- problem constraints.

Energy Management System First, we consider a real-world EMS that requires allocating minimum-cost power flows from different DERs [1]. The problem has a high level of uncertainty, which stems from uncontrollable deviations from the planned consumption load and the presence of Renewable Energy Sources. Based on actual energy prices, and forecasts on the availability of DERs and on consumption, the EMS decides: 1) how much energy should be produced; 2) which generators should be used; 3) whether the surplus of energy should be stored or sold to the energy market. The problem admits both a single-stage and a sequential formulation; in the former, a plan for 96 time units (each one 15 minutes long) must be prepared one day in advance; in the latter, routing decisions are made each time unit for the next one, until the end of horizon is reached.

In this case, historical costs, forecasts, and actual power generation and consumption represent the available data. The objective function is the power flow cost and the constraints impose power balance and power flow limits. This problem was tackled in [2] by introducing a virtual model parameter. In particular, it was shown how associating a (normally absent) cost to the storage equipment can improve the performance of a baseline optimization method. An effective, dedicated, algorithm configuration approach was then developed.

A complete model is provided in the supplemental material.

Set Multi-cover Second, we consider a simplified production planning problem, modeled as a Set Multi-cover Problem with stochastic coverage requirements [3]. Given a universe \( N \) containing \( n \) elements and a collection of sets over \( N \), the Set Multi-cover Problem requires finding a minimum size sub-collection of the sets such that coverage requirements for each element are satisfied. The sets may represent products that need to be manufactured together, while the coverage requirements represent product demands.

We consider a version of the problem where sets have non-uniform manufacturing costs, and where the demands are stochastic and unknown at production time. Unmet demands can then be satisfied by buying additional items, but at a higher cost. The requirements are generated according to a Poisson distribution, and we assume the existence of a linear relationships between an observable variable \( o \in \mathbb{R} \) and the Poisson rates \( \lambda_j = a_j o \quad \forall j \in N \).

In this case, the historical data is represented by a dataset \( \{ o_i, d_i \}_{i=1}^{m} \), where \( d \) are the demands and \( m \) is the dataset size. The objective is to minimize the cost of manufacturing and buying additional items; the constraints require to manufacture products in the same set together.

The full problem description is available in the supplementary material.
3 The UNIFY Framework

Our objective is to learn a policy that provides a high-quality solution to the problem itself. The term “policy” is a reference to Reinforcement Learning, which we will eventually employ; for sake of simplicity, however, we will first formalize the approach for single-stage problems, where all decisions must be taken at once.

Formally, let \( x \in X \) be a vector representing observable information and let \( z \) be a vector representing the decisions, which must come from the feasible set \( C(x) \). In the case of the EMS, \( x \) refers to the production and consumption forecasts and \( z \) are the power flow values. For the Set Multi-cover, the observable \( x \) corresponds to \( o \), whereas the decision variables \( z \) are the amount of sets to manufacture.

Typically, \( z \) will have a fixed size and \( C(x) \) will specify which vectors in the decision space are feasible. In general, however, even the size of \( z \) may depend on the observable (e.g. decide which transplants \( z \) to perform, given a pool \( x \) of patients and donors). In all cases, we aim at defining a function \( \pi(x, \theta) \), with parameter vector \( \theta \in \Theta \), such that:

\[
\pi : (x, \theta) \mapsto z \in C(x)
\]  

(1)

The \( \pi \) function is our constrained policy. In both the use cases, \( \pi \) should provide feasible decisions, i.e. power flow values or units of each set to be manufactured. We wish to choose \( \theta \) to minimize a cost metric on a target distribution. The corresponding training problem can be formalized as:

\[
\arg \min_{\theta \in \Theta} E_{(x_+, x)\sim p} \left[ f(x_+, x, \pi(x, \theta)) \right]
\]  

(2)

where \( f(x_+, x, z) \) is a function returning the cost of decisions \( z \), when \( x \) is observed and uncertainty unfolds with outcome \( x_+ \). We assume without loss of generality that \( x_+ \in X \); the term \( p \) refers to the training distribution (e.g. approximated via a simulator or a training set).

Given a solution \( \theta^* \) to the training problem, we can then perform inference (i.e. solve the decision problem) by observing \( x \) and evaluating \( \pi(x, \theta^*) \). Unfortunately, Equation (2) is hard to solve, since \( \pi \) will typically be trained on a large dataset and it is expected to always return feasible decisions from a space possibly lacking a fixed structure.

Our key insight is that Equation (2) can be made easier to handle by decomposing the policy into a traditional Machine Learning model and a traditional Constrained Optimization problem. Formally, the policy can be reformulated as:

\[
\pi(x, \theta) = g(x, h(x, \theta))
\]  

(3)

with:

\[
g(x, y) \equiv \arg \min_{z \in C(x, y)} \tilde{f}(x, y, z)
\]  

(4)

where \( h(x, \theta) \) is the ML model and \( g(x, y) \) is a function defined via the constrained optimization problem. The term \( y \), which corresponds to the output of the ML model, is referred to as virtual parameter vector. Its value may have an impact both on the feasible set \( C \) and on the cost \( \tilde{f} \) of the optimization problem, which are referred to as virtual feasible set and virtual cost. For example, in the EMS, \( y \) may correspond to the (normally absent) cost associated to the storage system mentioned in section 2 and as a side effect require to use a modified cost function \( \tilde{f} \). It is also possible to use an existing set of parameters as \( y \); for instance, in the Set Multi-cover use case, the ML model can be designed to predict the coverage requirements \( d \), thus requiring no modification in the structure of the feasible set.

Properties of the Approach   There are a few things to notice about Equation (3) and (4). First, in the reformulated policy it is comparatively easy to enforce feasibility and to deal with combinatorial decision spaces: since this is done outside of the ML model, any traditional constrained optimization method can be used (e.g. Mathematical Programming, Constraint Programming, or the Alternating Direction Method of Multipliers).

Second, the reformulated training problem is:

\[
\arg \min_{\theta \in \Theta} E_{(x_+, x)\sim p} \left[ f(x_+, x, z) \right]
\]

\[
z = g(x, y) = \arg \min_{z \in C(x, y)} \tilde{f}(x, y, z)
\]

\[
y = h(x, \theta)
\]  

(5)

This is a bilevel problem, combining unconstrained optimization on \( \theta \) and constrained optimization on \( z \). Several techniques are available to tackle Equation (5). For example, if \( h \) is differentiable, one may use the classical subgradient method to reach a local optimum: in the “forward pass” we evaluate \( h \) and compute \( z \), in the “backward pass” we fix the value of \( z \) and differentiate \( h \) w.r.t. the parameters \( \theta \).
While the original approach was limited to convex costs and constraints, subsequent works have tackled combinatorial problems, either in an approximate fashion via continuous relaxations, or in an exact fashion by assuming a fixed feasible space and linear costs. Outer and inner relaxations have also been used to improve scalability.

While this approach is viable, it misses a key opportunity: in fact, as the notation and terminology for the reformulated problem \( \tilde{C} \) and \( \tilde{f} \) imply, the feasible set and cost function of the inner optimization problem \( g \) may differ from the original ones. For example, it is possible to introduce penalties or rewards, buffers on constraint satisfaction thresholds, or even to relax constraints or to remove cost terms. This element of flexibility provides a new design handle that can be used to “partition” the challenging aspects of the original problem into either \( h \) or \( g \), depending on which of the two components is best suited to deal with them. While this is a powerful new mechanism to tackle complex problems, it does require a degree of creativity and expertise to be effectively used. We provide a few examples of how to do it in Section 5.

### Sequential Formulation and RL

The training formulation from Equation (5) applies to single-stage problems, but it can be extended to sequential decision-making. Formally, we can view the problem as a Markov Decision Process \( \langle X, Z, p, f, p_1, \gamma \rangle \) where \( X \) is the set of possible (observable) states and \( Z \) is the decision space, \( p_1 \) is the probability distribution for state transitions, \( f \) is the cost function, \( p_1 \) is the probability distribution for the initial state, and \( \gamma \in (0, 1] \) is a discount factor. At each step of the sequential process we will have access to a distinct observed state \( x_k \) and we will output a distinct decision vector \( z_k \); the value \( p_1(x_{k+1}, x_k, z_k) \) denotes the probability of reaching state \( x_{k+1} \) when applying decisions \( z_k \) on state \( x_k \); the cost function \( f \) is the same as in Equation (2) and (5). Within this framework, the training problem becomes:

\[
\arg\min_{\theta \in \Theta} \mathbb{E}_{\tau \sim p} \left[ \sum_{k=1}^{eoh} \gamma^k f(x_{k+1}, x_k, z_k) \right]
\]

\[
z_k = g(x_k, y_k) = \arg\min_{z \in \tilde{C}(x_k, y_k)} \tilde{f}(x_k, y_k, z_k)
\]

\[
y_k = h(x_k, \theta)
\]

where \( y_k \) is the ML model output for step \( k \), and \( \tau \) refers to a trajectory, i.e. to a sequence of states, ML outputs, and decisions \( \{(x_k, y_k, z_k)\}_{k=1}^{eoh} \). The probability of a trajectory is given by \( p(\tau) = p_1(x_1) \prod_{k=1}^{eoh} p_1(x_{k+1}, x_k, z_k) \). The term \( eoh \) is the End Of Horizon, and it can be infinite if the sequence is not upper-bounded. In this case, the discount factor \( \gamma \) should be strictly lower than 1, while \( \gamma \) should be equal to 1 for decision problems over a finite horizon.

Equation (6) can be interpreted as defining a Reinforcement Learning problem, where the \( h \) plays the role of a conventional RL policy, and \( g \) can be viewed at training time as part of the environment. This is an important observation since it implies that any RL approach can be used. Once an optimized parameter vector \( \theta^* \) has been obtained, the reformulated policy is given by \( g(x, h(x, \theta^*)) \) as usual. The sequential formulation directly generalizes the single step one, meaning that RL algorithms can be used to tackle Equation (5). In fact, this is exactly what we do in our experimentation since it simplifies the exposition.

### 4 Relation to Other Approaches

#### Decision Focused Learning (DFL)

Approaches in this class seek to train estimators for parameters of optimization models, while explicitly accounting for the impact that estimation inaccuracy has on the decisions. The idea gained attention after the seminal work by [4], with several new methods being proposed – and well covered in a recent survey by [5].

While the original approach was limited to convex costs and constraints, subsequent works have tackled combinatorial problems, either in an approximate fashion via continuous relaxations, or in an exact fashion by assuming a fixed feasible space and linear costs. Outer and inner relaxations have also been used to improve scalability.

DFL can be interpreted as solving (via subgradient optimization) a close variant of Equation (5), with some restrictions and one generalization. In particular, all DFL approaches lack virtual parameters: the ML model is instead expected to estimate part of the future state, i.e. \( y \) is a prediction for a portion of \( x_+ \). For example, the estimator might look at current traffic to predict future travel times. Additionally, \( \tilde{f} \) always corresponds to the original decision problem cost, and in all but a few cases the feasible space is fixed, i.e. \( C(x, y) = C \). The connection between \( y \) and \( x_+ \) implies that...
A first class of techniques attempts to learn within the same ML model how to satisfy the constraints and how to maximize the reward, similarly to what is done in the classical penalty method. Just as for the penalty method, using a large penalty is effective at enforcing constraint satisfaction, but can cause numerical instabilities and lead to poorly optimized policies. As a result, calibrating the penalty value is a non-trivial task. Another strategy, investigated by [13], enforces constraints by projecting the policy parameters in the pre-image of the feasible space. In other words, after a gradient update, a projection step adjusts the weights so that the decision vector becomes feasible, as in the projected gradient method [14]. This approach is more numerically stable, but also more computationally expensive.

Since all methods mentioned so far attempt to learn constraint satisfaction by changing the policy parameters, infeasible decisions may still occur on unseen examples due to generalization errors. For this reason, a second class of methods enforces constraint satisfaction via a projection step in decision space, rather than in weight space. In other words, once a baseline policy has provided a decision vector, this is projected in feasible space by minimizing a Euclidean distance. This step is often presented as a safety layer on top of a Neural Network policy [15]. This technique can guarantee constraint satisfaction, and it is more scalable than projection in weight space. However, projection can still lead to lower rewards.

The first class of approaches can be seen as approximately solving Equation (2). The second class can be assimilated to Equation (6), except that the ML output is already a decision vector (i.e. $y \in Z$), and that $\hat{f}(x, y, z)$ is always the Euclidean distance $\|y - z\|_2$. Our method therefore generalizes both classes of approaches. As the main appeal, the use of an arbitrary optimization problem in UNIFY frees the ML model from the need to output a decision vector, and opens up the possibility to solve a difficult task by partitioning its complexity between the model $h$ and the function $g$.

Algorithm Configuration Many approaches in the fields of Algorithm Configuration, Parameter Tuning, and Auto ML are concerned with adjusting the parameters of a given algorithm so as to optimize its behavior on a target distribution. A good survey is provided by [16]. For example, the approaches in [17][18] consist of surrogate-based black-box optimization procedures to select the parameters of a target algorithm, so as to maximize its performance on a given benchmark. A similar, but more rigorous, result is achieved in [19] for myopic online algorithms; the proposed technique is however only applicable to convex problems. Instance-specific configuration algorithms, such as the one from [20][21], have the same goal, but they are capable of selecting different parameter values depending on the properties of the input instance.

The Dynamic Algorithm Configuration (DAC) approach from [22] is capable of adjusting the parameter values as the target algorithm progresses, which can provide advantages for iterative optimization processes (e.g. gradient descent) and sequential decision making. DAC works by casting the configuration problem as a Contextual MDP and using RL to obtain a policy.

Traditional Algorithm Configuration methods can be interpreted as solving Equation (5), while DAC as solving the sequential formulation from Equation (6). In all cases but one, the vector $y$ corresponds to algorithm parameters (e.g. learning rates), rather than model parameters. Moreover, these approaches treat the algorithm to be configured as fixed, and therefore they do not take advantage of the flexibility offered by virtual parameters. To the best of our knowledge, the only applications of Algorithm Configuration together with true virtual parameters are provided by [23] for the Kidney Exchange Problem and [24] for an Energy Management System use case; however, these approaches have never been generalized.

Stochastic Optimization The area of Stochastic Optimization [25] also aims at improving robustness in single- or multi-stage decision-making problems.
Most stochastic optimization algorithms rely on Monte Carlo methods to approximate expected values and assess constraint satisfaction. The Sample Average Approximation (SAA) has long been a staple of the field; its convergence rate in the context of combinatorial problems was eventually provided in [26]. The SAA has been combined with Benders decomposition to address two-stage decision problems, leading to the family of L-shaped methods for stochastic optimization [27, 28]. Multi-stage (i.e. sequential) decision problems have been often approximated as a sequence of 2-stage problems in so-called online anticipatory algorithms [29], and solved once again via L-shaped methods. The connection between online stochastic optimization and Markov Decision Processes has been instead exploited directly by the AMSAA method from [30].

The stochastic optimization algorithms discussed here can be interpreted as addressing Equation (5), or Equation (6) in the case of AMSAA, without making use of a ML model, i.e. with $h(x, \theta) = x$. Because of that, there is no training step and solving a new instance requires approximating the expected value from scratch, making the process quite expensive. Our formulation suggests how by introducing a ML model the computational cost of sampling can be paid in a single offline phase, making inference much more efficient.

5 Empirical Evaluation

Our experimental evaluation is designed to show how UNIFY can be used to achieve different results, and how a decision problem can be refactored, assigning its parts to the most suitable component among $h$ or $g$. In particular, we use our approach to: 1) perform tuning of virtual parameters, similarly to Algorithm Configuration; 2) enforce constraint satisfaction in Reinforcement Learning; 3) obtain results analogous to DFL in a scenario where existing approaches are not applicable; 4) improve decision robustness without relying on the Sample Average Approximation.

5.1 Model Parameter Tuning

In this section, we approach model parameter tuning as an instance of UNIFY exploiting its properties, namely adding virtual parameters to the optimization model and framing the task as a sequential decision-making problem.

The EMS is a good candidate for this experiment since it has a straightforward sequential formulation. Moreover, the online optimization problem employed at each stage is suboptimal because it does not take into account the full-time horizon. Since the online optimal solver is myopic and suboptimal, we can improve its behavior by introducing a virtual cost parameter. Storing energy has no profit so the online (myopic) solver always ends up selling all the energy on the market. In particular, for this problem, we can define a virtual cost parameter related to the storage system (referred to as $c_{st}$), and it is possible to associate a profit (negative cost) with storing energy, which enables addressing this limitation. Intuitively, it is desirable to encourage the online solver to store energy in the battery system when the prices of the Electricity Market are cheap and the loads are low, in anticipation of future higher users’ demand.

In [31, 32], the authors develop TUNING, a hybrid offline/online optimization algorithm to find the optimal model parameters, but they assume a convex online optimization problem. Recently, [24] have explored the idea of using learning-based approximations as black-box solvers to perform model parameter tuning in a simpler integration scheme. In particular, their method employs Deep Reinforcement Learning as a black-box tool to find the optimal $c_{st}$ of the EMS described above.
In the following we will show that both the SINGLE-STEP and MDP methods proposed by [24] are instances of UNIFY. The former optimizes the parameters all at once, similarly to Algorithm Configuration approaches: according to Equation (5), the ML model \( h \) provides the virtual costs for all the stages, namely \( y = c_{1,...,96}^v \). Conversely, MDP exploits the sequential nature of the problem and, accordingly to Equation (6), the model output at each step \( k \) is \( y_k = c_k^v \). We refer to them respectively as UNIFY-SINGLE-STEP and UNIFY-SEQUENTIAL.

Similarly to [24], we compare the methods ensuring they have access to the same computation time. Since the time execution of TUNING is constant, we chose this value as time limit for the training of the other methods and plot it as a horizontal line. In Figure 1, we show the optimality gap w.r.t. the computation time. As also highlighted in [24], exploiting the sequential nature of the problem does not provide clear benefits (possibly due a suboptimal training solution) and UNIFY-SINGLE-STEP overcomes both TUNING and UNIFY-SEQUENTIAL.

5.2 Constraints in RL

Deep Reinforcement Learning (DRL) approaches have trouble dealing with combinatorial structures and hard constraints in general. Our UNIFY formulation provides a solution by delegating constraints satisfaction (and decision space exploration) to a second solver that can handle them more effectively. By doing so, the DRL algorithm can focus on a simpler task.

For this experiment we use again the EMS use case as a benchmark. The problem is challenging because a policy must satisfy hard instantaneous constraints at each stage, i.e. the flow bounds and the power balance constraints. We train a full end-to-end DRL algorithm to provide a solution, by learning constraints satisfaction only from the reward signal and refer to it as RL. The design of the reward function is not trivial because it should provide a good trade-off between finding good solutions and exploring the feasible space. Projection-based DRL algorithms (e.g. Safety Layer) provide an alternative to full end-to-end methods when dealing with constraints: we have experimented with a Safety Layer implementation for the EMS and we will refer to it as SAFETY-LAYER.

As shown in Section 4, both SAFETY-LAYER and UNIFY-SEQUENTIAL are instances of our UNIFY framework, but they have a critical difference: in SAFETY-LAYER the projection step can fix infeasible decisions, but this is done in a cost-agnostic fashion and the RL agent still needs to output a meaningful decision vector; conversely, in UNIFY-SEQUENTIAL the RL agent is indirectly guiding a problem-specific solver, which has the same guarantees in terms of feasibility, but it is arguably a simpler task.

In the upper and lower parts of fig. 2, we respectively show the optimality gap of all the methods and the number of failed episodes of RL due to constraints violations. In the early stages of training, RL never completes a full episode. It then progressively learns to satisfy constraints but, conversely, the cost of the solutions found increases. On the other hand, SAFETY-LAYER converges very quickly but the final solution cost is very close to the one provided by RL. UNIFY-SEQUENTIAL quickly converges as well, and it also improves the previous methods of a non-negligible gap.
These experimental results demonstrate that Reinforcement Learning can benefit from a policy reformulation that properly balances learning and optimization.

**Generalization of DFL**  In this section, we will show that UNIFY can be used in place of classical Decision Focused Learning approaches.

For this experiment, we will consider the Set Multi-cover Problem with stochastic coverage requirements and make a comparison with a traditional predict-then-optimize approach. In the UNIFY formulation for this use case, the RL policy predicts the coverage requirements, \( y = \{ d_j \} \forall j \in N \) that are then plugged into the optimization model, and the overall policy is trained to minimize the solution cost. The UNIFY implementation is straightforward, whereas applying traditional Decision Focused Learning approaches is not trivial since the cost function is non-linear and non-differentiable. In the predict-then-optimize approach, we first train a ML model to accurately predict the rates of the underlying Poisson distribution that generates the stochastic coverage requirements, and then we use the predicted rates as the requirements in the Set Multi-cover optimization model.

![Figure 3: Here we report the predicted \( \lambda \) MAPE of the Machine Learning model employed in the predict-then-optimize approach.](image3)

For training and testing the methods, we used two separated sets of instances. As we can see in fig. 3, the Mean Absolute Percentage Error (MAPE) for each of the rate \( \lambda_i \forall i \in I \) is low, proving that the ML model is accurate. Despite this fact, as shown in fig. 4, the true task loss, i.e. the solution cost, is far from optimal. On the other side, the UNIFY implementation that is trained to directly minimize the task loss greatly outperforms the predict-then-optimize approach and it is considerably closer to the optimal cost. We can thus conclude that UNIFY is a valid alternative to traditional Decision Focused Learning approaches, when those cannot be easily applied.

![Figure 4: This figure reports the mean cost and standard deviation for the UNIFY and the Predict-then-optimize approaches compared to the optimal values.](image4)

5.3 Stochastic Optimization

Solving stochastic optimization problems can be incredibly challenging. As mentioned in section 4, SAA methods are widely adopted in this field but they can be computationally expensive. In this section we will show how UNIFY can be used to improve the robustness of the downstream solver by performing a set of experiments on the Set Multi-cover with stochastic coverages.
As a baseline approach, we implemented a SAA method that computes the optimal solution on a fixed set of instances (referred to as training instances). As also described in section 4, this approach is a very simple instance of UNIFY without the Machine Learning component: it basically ignores the relationship between the observable variable $x$ and the Poisson rates $\lambda$. We also provide a more robust baseline method that relies on the predict-then-optimize framework: we train a Machine Learning model on the training instances to estimate the parametrization of the probability distribution that models the uncertain variables; we then exploit the model predictions to generate samples for the downstream optimization model. Finally, we also train a more advanced implementation of UNIFY, where the RL policy predicts the demands and the overall policy is trained to minimize the task loss, the same as described in the previous paragraph; notably, the latter approach does not rely on sampling. It is worth highlighting that the comparison favors the SAA method, since it is designed by assuming exact knowledge of the type of probability distribution; the UNIFY implementation makes no such assumption.

![Normalized cost](image1)

![Normalized runtime](image2)

Figure 5: Optimality gap of the three methods on the Set Multi-cover problem with stochastic demands and the solution time of the predict-then-optimize approach w.r.t. the number of scenarios.

Results are shown in fig. 5. In the upper part of the figure, we report the optimality gap of the three methods on a separated set of instances w.r.t. the number of sampled scenarios. Both the simple SAA algorithm and predict-then-optimize approaches benefit from increasing the number of sampled scenarios. On the other side, the UNIFY implementation does not depend on the number of sampled scenarios, because it directly predicts the coverage values that are then plugged into the optimization model. Despite the advantage previously discussed, the predict-then-optimize approach surpasses UNIFY only when at least $\sim 50$ scenarios are used in the downstream stochastic optimization model. In the lower part of the figure, we show the runtime required by predict-then-optimize as a multiple of the runtime of UNIFY, w.r.t. to the number of scenarios. As we can see, to obtain better results, predict-then-optimize requires more than 200 times the computation of UNIFY.

We can thus conclude that a smart implementation of UNIFY is a cheaper alternative to a SAA method for improving the robustness of the solver when facing stochastic optimization problems.

### 6 Concluding Remarks

In this paper we proposed UNIFY, a flexible framework for solving CO problems with ML. At the price of a higher design effort, we can face complex problems more easily by reformulating the original policy in two components: a ML model and a traditional constrained optimization problem. We showed that UNIFY provides a unified view of several approaches, which we hope will improve cross-fertilization by highlighting previously unrecognized connections. Finally, we performed an extensive experimental evaluation of two practical problems to highlight the benefits of the approach.

Several open questions remain and we hope they will encourage future works in this direction. As mentioned in section 4, UNIFY is still not a complete generalization of DFL and we should find a way to adapt surrogate losses defined by DFL methods in UNIFY. In addition, Reinforcement Learning has been recently employed to build a solution for combinatorial optimization problems or inside the search process of already existing solvers. With some effort, it may be possible to reformulate these methods in the UNIFY framework.
Despite the degree of success obtained in recent years, Reinforcement Learning has still some issues that limit its applicability on real-world problems. To name one of them, Reinforcement Learning is sample inefficient [33]: it requires several interactions with the environment before reaching convergence. It could be interesting to investigate whether improving the communication of the two UNIFY components can lead to faster convergence at training time.

Problems where the decision space changes depending on the observable variables or where constraints are defined over multiple steps are challenging for traditional DFL approaches. As part of future works, we would like to study how UNIFY can be used to face this kind of problem.
A Set Multi-cover with stochastic coverage requirements

We start from the formulation of the deterministic version of the problem:

\[
\min \sum_{j \in J} c_j x_j \tag{7}
\]

\[
\sum_{j \in J} a_{i,j} x_j \geq d_i \quad \forall i \in I \tag{8}
\]

\[
x_j \geq 0 \tag{9}
\]

\[
x_j \in \mathbb{Z} \tag{10}
\]

\[
a_{i,j} \in \{0, 1\} \tag{11}
\]

where \( I \) is the universe, \( J \) is the collection of all possible sets, \( a \) is the availability matrix, \( d_i \) is the required coverage for the \( i \)-th element of the universe, \( c_j \) is the cost of the \( j \)-th set and \( x \) is the vector of decision variables.

In the stochastic version of the problem, the coverage requirements are sampled from a Poisson distribution with rate \( \lambda_i \) \( \forall i \in I \), namely \( d_i \sim \text{Poisson}(\lambda_i) \).

Stochastic optimization model As a baseline method to solve the Set Multi-cover with stochastic coverages, we implemented a Sample Average Approximation (SAA) algorithm based on Monte Carlo sampling.

The optimization model is defined in the following way:

\[
\min \sum_{j \in J} c_j x_j + \frac{1}{|\Omega|} \sum_{\omega \in \Omega} \sum_{i \in I} w_{i,\omega} s_{i,\omega} \tag{12}
\]

\[
\sum_{j \in J} a_{i,j} x_j \geq d_{i,\omega}(1 - z_{i,\omega}) \quad \forall i \in I, \omega \in \Omega \tag{13}
\]

\[
z_{i,\omega} = 1 \implies s_{i,\omega} \geq d_{i,\omega} - \sum_{j \in J} a_{i,j} x_j \quad \forall i \in I, \omega \in \Omega \tag{14}
\]

\[
x_j \geq 0 \tag{15}
\]

\[
z_{i,\omega} \in [0, 1] \tag{16}
\]

\[
s_{i,\omega} \geq 0 \tag{17}
\]

\[
x, z \in \mathbb{Z} \tag{18}
\]

where \( \omega \in \Omega \) are the sampled scenarios, \( w \) is the penalty vector due to the violation of the coverage requirements constraints of eq. (13), \( z \) is a vector of indicator variables that allow violation of eq. (13) and \( s \) is a vector of slack variables that keep track of the not satisfied demands.

Energy Management System An Energy Management System (EMS) requires the allocation of the minimum-cost power flows from different Distributed Energy Resources (DERs). The uncertainty stems from uncontrollable deviations from the planned loads of consumption and the presence of Renewable Energy Sources (RES). Based on actual energy prices and on the availability of DERs, the EMS decides: 1) how much energy should be produced; 2) which generators should be used for the required energy; 3) whether the surplus energy should be stored or sold to the energy market. Unlike in most of the existing literature, we acknowledge that in many practical cases some parameters can be tuned offline, while in most of the energy balance should be maintained online by managing energy flows among the grid, the renewable and traditional generators, and the storage systems. Intuitively, handling these two phases in an integrated fashion should lead to some benefits, thus making the EMS a good benchmark for our integrated approach.

In our case study, it is desirable to encourage the online heuristic to store energy in the battery system when the prices of the Electricity Market are cheap and the loads are low, in anticipation of future higher users’ demand. Storing energy has no profit so the online (myopic) solver always ends up selling all the energy on the market. However, by defining a virtual cost parameter related to the storage system, it is possible to associate a profit (negative cost) with storing energy, which enables addressing this greedy limitation. Then, based on day-ahead RES generation and electric demand forecasts, we can find the optimal virtual costs related to the storage system to achieve better results in terms of solution quality (management costs of the energy system).
B State-of-the-art Offline/Online approach

We refer to TUNING as the integrated offline/online optimization method proposed in [2] that assumes exogenous uncertainty, and that is composed of two macro steps: an offline two-stage stochastic optimization model based on sampling and scenarios; and an online parametric algorithm, implemented within a simulator, that tries to make optimal online choices, by building over the offline decisions. The authors assume that the online parametric algorithm is based on a convex optimization model. Based on some configuration parameters of the online model, an offline parameter tuning step is applied. In this way, the authors can take advantage of the convexity of the online problem to obtain guaranteed optimal parameters. In particular, convexity implies that any local minimum must be a global minimum. Local minima can be characterized in terms of the KKT optimality conditions. Essentially, those conditions introduce a set of constraints that must be satisfied by any solution that is compatible with the behavior of the online heuristic. They can exploit this property by formulating the tuning phase as a Mathematical Program that is not a trivial task for every constrained real-world problem.

The online step is composed by a greedy (myopic) heuristic that minimizes the cost and covers the energy demand by manipulating the flows between the energy sources. We underline that this is a typical approach to handle the online optimization of an EMS [1]. The heuristic can be formulated as an LP model:

\[
\begin{align*}
\min & \sum_{k=1}^{n} \sum_{g \in G} c_g^k x_g^k \\
\text{s.t.} & \quad \hat{L}^k = \sum_{g \in G} x_g^k \\
& \quad 0 \leq \gamma_k + \eta x_0^k \leq \Gamma \\
& \quad \underline{x}_g \leq x_g^k \leq \bar{x}_g 
\end{align*}
\]  

For each stage \( k \) up to \( n \), the decision variables \( x_g \) are the power flows between nodes in \( g \in G \) and \( c_g \) are the associated costs. All flows must satisfy the lower and upper physical bounds \( \underline{x}_g \) and \( \bar{x}_g \). Index 0 refers to the storage system and the index 1 to the RES generators. Hence the virtual costs associated with the storage system are \( c_0^k \). The battery charge, upper limit and efficiency are \( \gamma, \Gamma \) and \( \eta \). The EMS must satisfy the user demand at each stage \( k \) referred to as \( \hat{L}^k \).

The baseline offline problem is modeled via MIP and relies on the KKT conditions to define a model for finding the optimal values of \( c_0^k \) for the set of sampled scenarios \( \omega \in \Omega \). Such model is given by:

\[
\begin{align*}
\min & \frac{1}{|\Omega|} \sum_{\omega \in \Omega} \sum_{g \in G} \sum_{k=1}^{n} c_g^k x_g^k \\
\text{s.t.} & \quad \hat{L}_\omega^k = \sum_{g \in G} x_g^k \quad \forall \omega \in \Omega, \forall k = 1, \ldots, n \\
& \quad \underline{x}_g \leq x_g^k \leq \bar{x}_g \quad \forall \omega \in \Omega, \forall k = 1, \ldots, n \\
& \quad 0 \leq \gamma^k \leq \Gamma \quad \forall k = 1, \ldots, n \\
& \quad \gamma^{k+1} = \gamma^k + \eta x_0^k \quad \forall \omega \in \Omega, \forall k = 1, \ldots, n - 1 \\
& \quad x^{k+1} = \hat{R}_k + \xi_{R,\omega} \quad \forall \omega \in \Omega, \forall k = 1, \ldots, n \\
& \quad \hat{L}_\omega^{k+1} = \hat{L}_\omega^k + y_k + \xi_{L,\omega} \quad \forall \omega \in \Omega, \forall k = 1, \ldots, n 
\end{align*}
\]

\( \hat{R}_k \) and \( \hat{L}_k \) are the estimated RES production and load, and \( \xi_{R}^{k} \) and \( \xi_{L}^{k} \) are the corresponding random variables representing the prediction errors. \( y_k \) are optimal load shifts and are considered as fixed parameters. The authors assume that the errors follow roughly a Normal distribution \( \mathcal{N}(0, \sigma^2) \) and that the variance \( \sigma^2 \) is such that 95% confidence interval corresponds to \( \pm 10\% \) of the estimated value. \( \hat{L}_\omega^k \) is the observed user load demand for stage \( k \) of the scenario \( \omega \). Equations (27) to (29) model the transition functions.

The above formulation is free to assign variables (as long as the constraints are satisfied), whereas all decisions that are supposed to be made by the heuristic can not rely on future information. The authors account for this limitation by introducing, as constraints, the KKT optimality conditions for the convex online heuristic. The model achieves integration at the cost of offline computation time, because of the additional variables introduced and the presence of non-linearities.
In the following we show the KKT conditions formulation for the online heuristic in a single scenario:

\[-c_k^g = \lambda_k^g + \mu_{k,g,\omega}^g - \nu_{k,g,\omega}^g \quad \forall g \in G \tag{30}\]

\[\mu_{k,g,\omega}^g (x_{k,g,\omega}^g + \pi_g) = 0 \quad \forall g \in G \tag{31}\]

\[\nu_{k,i,\omega}^g (x_g - x_{g,\omega}^i) = 0 \quad \forall g \in G \tag{32}\]

\[\hat{\mu}_{k,\omega}^g (\eta x_{k,0,\omega}^g + \gamma^k - \Gamma) = 0 \tag{33}\]

\[\hat{\nu}_{k,\omega}^g (\eta x_{k,0,\omega}^g + \gamma^k) = 0 \tag{34}\]

\[\mu_{k,g,\omega}^g, \nu_{k,g,\omega}^g \geq 0 \quad \forall g \in G \tag{35}\]

\[\hat{\mu}_{k,\omega}^g, \hat{\nu}_{k,\omega}^g \geq 0 \tag{36}\]

where \(\mu_{k,g,\omega}^g\) and \(\nu_{k,g,\omega}^g\) are the multipliers associated to the physical flow bounds, while \(\hat{\mu}_{k,\omega}^g\) and \(\hat{\nu}_{k,\omega}^g\) are associated to the battery capacity bounds. Injecting the conditions in the offline model yields:

\[
\min \frac{1}{|\Omega|} \sum_{\omega \in \Omega} \sum_{g \in G} \sum_{k=1}^{n} c_k^g x_{k,g,\omega}^g \\
\text{s.t. Eq. (24)} - (29) \quad \text{Eq. (30)} - (36) \quad \forall \omega \in \Omega, \forall k = 1, \ldots n
\]

where the decision variables are \(x_{k,g,\omega}^g\), \(\mu_{k,g,\omega}^g\), \(\nu_{k,g,\omega}^g\), \(\hat{\mu}_{k,\omega}^g\), \(\hat{\nu}_{k,\omega}^g\). To those, the authors add the cost \(c_k^0\) associated with the flow from and to the storage system (the only parameter they allow the solver to adjust). This method allows the offline solver to associate a virtual profit for storing energy, which enables addressing the original limitation at no online computational cost.

### C Datasets

In this section we describe the datasets used to conduct our experimental evaluation.

**Energy Management System** For the EMS we used the same dataset of [24] that relies on real data based on a Public Dataset\(^2\). From this dataset, we assume electric load demand and photovoltaic production forecasts, upper and lower limits for generating units and the initial status of storage units. The realizations of uncertain variables, namely \(\tilde{R}\) and \(\tilde{L}\), are obtained from the forecasts by adding noise from a normal distribution as described in appendix B. The dataset presents individual profiles of load demand with a time step of 5 minutes resolution from 00:00 to 23:00. We consider aggregated profiles with a timestamp of 15 minutes and use them as forecasted load. The photovoltaic production is based on the same dataset with profiles for different sizes of photovoltaic units but the same solar irradiance (i.e. the same shape but different amplitude due to the different sizes of the panels used). Also in this case photovoltaic production is adopted as a forecast.

The electricity demand hourly prices have been obtained based on data from the Italian national energy market management corporation\(^3\) (GME) in €/MWh. The diesel price is taken from the Italian Ministry of Economic Development\(^4\) and is assumed as a constant for all the time horizon (one day in our model) as assumed in literature [1] and from [34].

For the evaluation, we randomly select 100 pairs of load demand and photovoltaic production forecasts.

**Set Multi-cover with stochastic coverages** For the Set Multi-cover with stochastic coverages, we generate the availability matrix \(a\) following the guidelines of [35]: every column covers at least one row and every row is covered by at least two columns. In addition, the availability matrix has a density (number of 1 in the matrix) of 2%. The set costs are randomly generated in the range \([1, 100]\) with a uniform probability distribution. The penalties \(w\) introduced in appendix A are computed as follows:

\[w_{i,\omega} = \max_{j \in J} c_j \cdot 10 \quad \forall \omega \in \Omega\]

\(^2\)www.enwl.co.uk/lnvns

\(^3\)http://www.mercatoelettrico.org/En/Default.aspx

\(^4\)http://dgsaie.mise.gov.it/
We generate 1000 instances with 200 elements and 1000 sets and we equally split them between training and test sets. The Poisson vector rates $\lambda$ is generated according to a linear relationship with an observable variable $o \in \mathbb{R}$, $\lambda = a_i o \\forall i \in I$. The coefficients $a_i$ and the observable variables vectors $o$ are randomly generated with an uniform probability distribution respectively in the range $[1, 5]$ and $[1, 10]$.

### D Reinforcement Learning Environments

In this section we provide a description of the environments design for the EMS and the Set Multi-cover with stochastic coverage requirements, namely observations, actions and reward function.

**Energy Management System** In the EMS use case we employed the same environment variants introduced in [24]. For UNIFY-SINGLE-STEP the observations are the day-ahead photovoltaic generation $\hat{R}^k$ and electric demand forecasting $\hat{L}^k$ and the actions are the set of virtual costs for all the stages $c_i^k$ for $k = \{1, \ldots, n\}$ and thus the policy is a function $\pi : \mathbb{R}^{n \times 2} \rightarrow \mathbb{R}^n$. Once $c_i^k$ are provided, a solution $\{x_g^k\}_{k=1}^n$ is found solving the online optimization problem defined in Equations (19) to (22) and the reward is the negative real cost computed as:

$$\sum_{k=1}^n \sum_{g \in G} \sum_{g \neq 0} \frac{c_i^k - c_g^k x_g^k}{g}$$

For UNIFY-SEQUENTIAL the policy $\pi$ is a function $\pi : \mathbb{R}^{n \times 3+1} \rightarrow \mathbb{R}$. The state $s_k$ keeps track of the battery charge $\gamma^k$ and it is updated accordingly to the input and output storage flows. At each stage $k$, the agent’s action $a_k$ is the virtual cost $c_i^k$ and the corresponding online optimization problem is solved. Then the environment provides as observations the battery charge $\gamma^k$, the set of forecasts $\hat{R}^k_{1\ldots n}$ and $\hat{L}^k_{1\ldots n}$, and a one-hot encoding of the stage $k$. The reward is again the negative real cost but for the only current stage $k$:

$$\sum_{g \in G} \sum_{g \neq 0} c_i^k x_g^k$$

In the full end-to-end Reinforcement Learning approach, the policy provides a $(|G| - 1)$-dimensional vector corresponding to the power flows for a single stage. The actions are clipped in the range $[-1, 1]$ and then rescaled in their feasible ranges $[\alpha_0, \alpha_1]$. Since one of the power flows has no upper bound $\alpha_0$, the authors have set its value so that the power balance constraint of eq. (23) is satisfied, reducing the actions space and making the task easier. We refer to this decision variable as $x_2^k$. Despite adopting these architectural constraints, the actions provided by the agent may still be infeasible: the storage constraint of eq. (23) and the lower bound $x_2$ can be violated. The reward is non-zero only for the last stage and it is computed as the negative cumulative real cost. Since the cost of the solution is in the range $[0, 3000]$, the policy network is rewarded with a value of $-10000$ when infeasible actions are selected to encourage the search for feasible solutions.

As last detail, for all the environments described above the observations are rescaled in the range $[0, 1]$ dividing by their maximum values.

**Set Multi-cover with stochastic coverages** For this use case, the environment has a single step duration: it provides the observable variable $o$ to the agent and the actions are the predicted coverages. The policy is thus a function $\pi : \mathbb{R} \rightarrow \mathbb{Z}$ where $I$ is the set of the elements. Since the Reinforcement Learning agent outputs real numbers, we convert its actions to the closest integer values. The reward is computed as the negative total cost:

$$- \sum_{j \in J} c_j \hat{x}_j - \sum_{i \in I} w_i \bar{d}_i$$

$$\bar{d}_i = \max \left( 0, d_i - \sum_{j \in J} a_{i,j} \hat{x}_j \right)$$

where $\hat{x}$ is the solution found using the predicted demands, $\bar{d}$ is the vector of not satisfied demands and $w$ is the vector of penalties as illustrated in appendix A.
E  Training and hyperparameter configuration

As Reinforcement Learning algorithm we employed the Advantage Actor-Critic (A2C)\textsuperscript{5} because it is robust and can deal with continuous actions space. Since hyperparameter search was outside the scope of the paper, we chose a quite standard architecture. The policy is represented by a Gaussian distribution for each action dimension, parametrized by a feedforward fully-connected Neural Network with two hidden layers, each of 32 units and a hyperbolic tangent activation function. The critic is again a deep neural network with the same hidden architecture of the policy.

Parameters are updated using Adam optimizer. For the experiments on the EMS use case, we opted for a learning rate of 0.01 (larger than usual) because it improved the convergence speed without compromising the final results.

For UNIFY-SINGLE-STEP in the EMS use case and the UNIFY implementation for the Set Multi-cover, we used a batch size of 100 whereas for UNIFY-SEQUENTIAL, RL and SAFETY-LAYER we preferred a larger batch size of 9600 to have a comparable number of episodes for each training epoch.

For the EMS experiments, UNIFY-SINGLE-STEP, UNIFY-SEQUENTIAL, RL and SAFETY-LAYER have been trained for respectively 37, 19, 52 and 19 epochs. We chose these values because we want to provide the same computation time required by TUNING algorithm. The UNIFY implementation for the Set Multi-cover was trained for 10000 epochs.

Experiments on the EMS were performed on a laptop with an Intel i7 CPU with 4 cores, 1.5 GHz clock frequency and 16 GB of memory. Experiments on the Set Multi-cover were conducted on a AMD EPYC 7272 16-Core Processor with 2.8 GHz clock frequency and 512 GB of memory. Despite the availability of multi-core processors, we do not exploit multi-threading and all experiments were executed on a single core to keep things the simplest as possible and simplify reproducibility.

\textsuperscript{5}A2C algorithm was implemented with the TensorFlow version of the garage \cite{garage} library.
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