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Optimath-X: An Explainable AI- Driven Mathematical Optimization Framework for Intelligent Decision - Making and Complex Problem Solving

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Abstract- Optimization algorithms in mathematics are key tools in the process of decision-making in engineering, logistics, and resources management, but traditional solvers operate like black boxes and provide no insights into how their solutions are obtained and on what grounds particular decisions are made. This lack of transparency is problematic for adopting the tool in contexts, where decision-makers have to be convinced before they make a move based on solver's suggestions. In this paper, we introduce an explainable AI-based optimization framework OptiMath-X, which unites surrogate-assisted metaheuristic search with explanation generation for mathematical optimization. The approach combines an evolutionary–local search solver with a consistent local explanation generator, which is constrained by problem structure and dependencies between variables. The experiments, conducted using benchmark problems and real-world instance from logistics domain show that our approach provides quality of solutions comparable to traditional solvers, and generated explanations are found useful by domain experts.

Key Word: Explainable Optimization, Mathematical Programming, Metaheuristics, Decision Support Systems, Local Explanations, Hybrid Search

I. INTRODUCTION

Optimization lies at the core of computational decision-making in today's world, helping businesses make allocation and scheduling decisions, designing systems and processes under conflicting objectives and constraints. The solutions computed through optimization methods have real-world implications, both operational and economic. As more and more business decisions are being made through artificial intelligence, there is a growing need for such decisions to be transparent. Operations managers, regulatory bodies, and other stakeholders need to know not only what is the suggested decision but why such a decision is better than alternative solutions [1].

The problem here is systemic. Traditional mathematical programming solvers whether simplex-based LP solvers or branch-and-bound integer programming solvers – focus on the efficiency and optimality of the solution rather than its transparency. While solving a mathematical programming model, a solver generates a lot of intermediate information which includes pivot operations, branching decisions and dual variables which are not accessible to non-expert users. Such a lack of transparency becomes even more complicated when machine learning is involved in the optimization process or the solution method used is some form of metaheuristic for problems which cannot be solved using exact methods [3], [7]. Explainable artificial intelligence (XAI) has been conceived as a response to the same lack of transparency in machine learning, giving rise to approaches like LIME, SHAP, and counterfactual explanations that shed light on how the model operates. But these approaches have been devised specifically for predictive models and ignore the unique nature of optimization problems in terms of hard constraints, dependency among variables, and

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the way solutions are built step by step. Using these conventional XAI approaches in optimization problems is highly likely to yield explanations that are mathematically inconsistent, implying variable perturbations that are not feasible or assigning importance to parameters inaccurately [1], [2], [6].
In this paper we present a novel framework called OptiMath-X which can overcome such limitations by incorporating explanation generation capability within the optimization loop. The contributions of the framework include

- A hybrid search strategy which utilizes a combination of population-based exploration and local optimization that results in solution trajectories carrying more information about the search process compared to traditional single-shot solving methods
- An integrated local explanation module which can generate feature-attribution explanations in such a way that they respect the structural constraints defined by the optimization model
- A modular framework that can handle problems with either continuous or discrete decision variables

The importance of this research lies beyond the technical novelty itself, and in line with the current trends in AI development, there is no doubt that the necessity for the ability to explain the rationale behind the results generated by the models becomes even more critical as the complexity and importance of optimization models increase [1], [5].

II. LITERATURE SURVEY

Recent studies have highlighted the connection between explainability and optimization, realizing the significance of the algorithmic decisions made in operations research that can be compared to those made in machine learning. In a systematic review of explainable AI in decision-making systems, Danach et al. observed that, despite several techniques like surrogate modeling, feature attribution, and rule extraction, interpretability is being embedded in optimization pipelines, but that there is a lack of integration of the techniques into the problem-solving procedure, meaning that most of the solutions do not consider the math behind the optimization problem [1].

Another important line of research is that related to the adaptation of local explanation methods for optimization applications. In this regard, CLEMO framework introduced by researchers dealing with coherent local explanations for mathematical optimization can be viewed as an answer to the aforementioned need, since it expands LIME's idea of generating explanations based on perturbations with the use of conditions which ensure the structural coherence between explanations and the affine and convex nature of the model in question [2]. CLEMO shows that it is possible to generate solver-agnostic explanations without sacrificing the fidelity of the model structure, although it is highly dependent on perturbation-based sampling, thus being less scalable in higher dimensions. Additionally, another interesting line of research is that involving counterfactual explanations for power grid optimization. In this context, researchers have proposed a framework allowing one to identify the infeasibility and propose demand-response actions [6].

The explainability of metaheuristic optimization has been studied in a different way in which one is trying to understand the algorithm itself and not just its solution. In the systematic study of the explainability of computational intelligence for optimization, it is stated that the metaheuristic algorithms (especially the evolutionary and swarm-based algorithms) have inherent opacity in their search mechanism and that landscape analysis and quality diversity can be used as approaches to help understand their search process [3]. The term “Explainergy” is introduced for the field of energy with the idea that domain-specific approaches to explanation are required for energy systems since generic XAI approaches do not account for the limitations.

The combination of machine learning algorithms and metaheuristic search strategies has led to the emergence of hybrids that help improve both the effectiveness and the explanation capabilities of optimization. In recent research on the hybrid fruit fly and bison optimization with reinforcement

learning, it was shown that surrogate models may cut down the costs of computations while giving some feature importance information for helping to navigate the search [4]. Moreover, the SIRO algorithm uses the components of machine learning to perform the initialization and configuration of parameters more intelligently [7].

Explanation in important engineering applications has become one of the most challenging problem domains. Scientific research dedicated to explainable and secure AI for defense, aerospace, and autonomy emphasizes the importance of transparency when the optimization result directly impacts safety and success of the mission and claims that explainability needs to be defined at design time and not added as an afterthought [5].

These views correspond to the results achieved in production planning applications, where methods of fuzzy evolving DL-XAI have been created to provide manufacturers with local and contrastive explanations in the context of centralized planning systems [8].

In general, the reviewed literature points out that explainable optimization is no longer only a matter of theoretical discussion but is becoming an engineering challenge, although integrated solution-explanation frameworks are still lacking [1], [3].

III. PROPOSED METHODOLOGY

1. Framework Architecture Overview

The system OptiMath-X works as a modular pipeline that has three distinct layers, which are the Problem Interface Layer that receives optimization model formulations such as objective functions, constraints, variables domain, and structural information; the Hybrid Optimization Engine that runs a hybrid evolutionary and local search algorithm; and the Explanation Generation Layer that generates explanations from the trajectory of the solution process and the formulation of the problem. Figure 1 shows the architecture of the whole system.

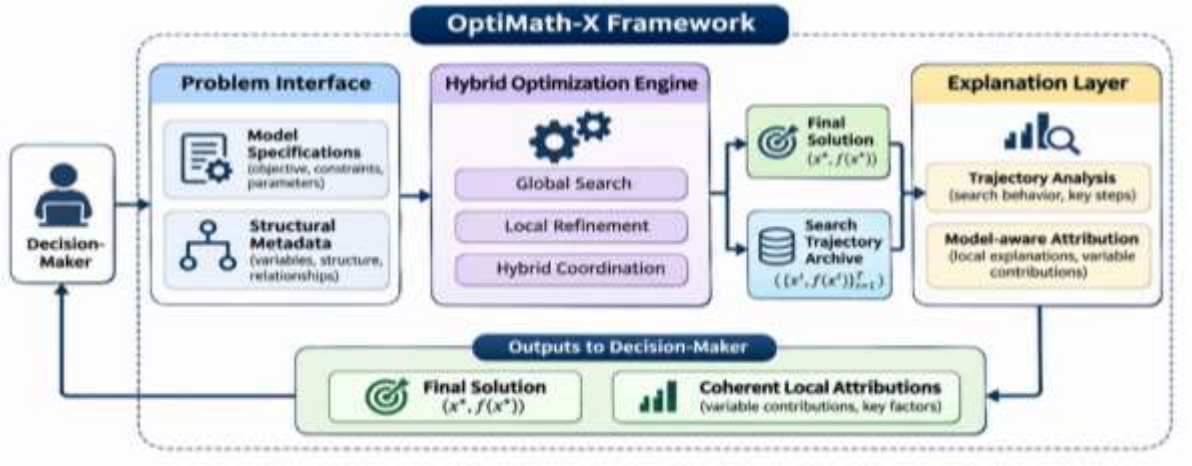

Figure 1. OptiMath-X framework architecture

It is an important architectural choice for explanation to be coupled with optimization and not to treat them as separate phases since explanations created directly during the search are more representative of the actual solver behavior than explanations generated after the optimization using only the inputs and outputs. The approach ensures preservation of information lost by one shot solver output.

Problem Representation and Structural Metadata

It allows for optimization problems to be formulated in a standard way, encompassing both their mathematical definition and their structural properties. In an optimization problem with decision variable $x \in \mathbb{R}^n$, objective function f(x), and feasible

set $\mathcal{C}$, the standard representation comprises: type annotations for each variable (continuous, integer, binary); information about the incidence of constraints on the decision variables; and the form of the objective function (linear, quadratic, interactions). This additional information is used in two ways for optimization and explanation generation.

For consistent explanation generation, the incidence structure becomes especially important. As the explanation generation module perturbs the values of certain variables, it uses the incidence matrix to verify that the perturbation does not violate any constraints on the variables and leaves the resulting perturbed sample feasible with regards to coupling constraints. This way, explanations are prevented from assigning importance to a variable that cannot be independently perturbed due to equality constraints—a typical problem encountered while using LIME naively on optimization problems.

3. Hybrid Optimization Engine

The optimization module uses two-phase search mechanism. In Phase 1, the evolutionary approach based on population where problem-specific encoding scheme is used: continuous variables are evolved using differential evolution scheme whereas the discrete variables can be evolved using swap and insertion neighborhoods for permutation/selection problem. Population initialization will be done using Latin hypercube sampling for continuous part and heuristics greedy construction for discrete part so that population covers the whole feasible region.
In Phase 2, it triggers when convergence stagnation occurs within population and is determined by checking moving average of objective improvement over a sliding window. Then, the local search mechanism is used to refine the best solutions from the incumbent solutions using neighborhood mechanisms according to the variable type: gradient search when continuous and differentiable and k-exchange for discrete variables. In this way, both exploration and exploitation are done along with generation of diverse trajectories which will be used as input in the explanation phase.

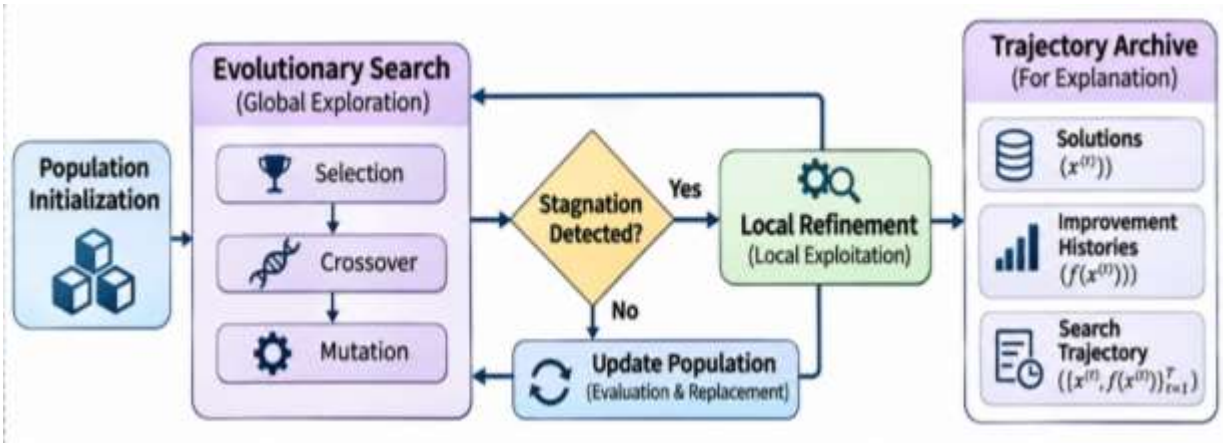

Figure 2. Hybrid search workflow within the optimization engine

The trajectory archive contains, for each population generation and for each local search operation, the following elements: the incumbent solution vector, its corresponding objective function value, any constraint violation (if there is one), and the operator used to create that particular solution vector. The trajectory archive is the evidence upon which explanations are generated.

4. Coherent Local Explanation Generation

The explanation component generates explanations based on feature attribution to a solution x using a local surrogate model in the vicinity of x. In contrast to classical LIME, the sample generation process is conditioned upon the structural metadata, meaning that all possible candidate perturbations violating coupling constraints and variable bounds are

discarded or mapped to the feasible domain before being evaluated. The surrogate model is a ridge regression on the original space of variables.

Formally, given solution x and a set of perturbed feasible samples $\{x^{(1)}, \ldots, x^{(M)}\}$ with corresponding objective values $\{y^{(1)}, \ldots, y^{(M)}\}$, the explanation module solves:

$$\beta = \text{argmin}_\beta \Sigma_i w_i (y^{(i)} - \beta^T x^{(i)})^2 + \lambda \|\beta\|^2$$

where $w_i = \exp(-\|x^{(i)} - x\|^2 / \sigma^2)$ provides weights based on proximity, and λ is the regularization term. The vector of coefficients β thus obtained expresses how much a given decision variable affects the objective function value, per unit change from x, assuming the local linearization holds true. If a decision variable takes on discrete values and the binary or categorical encoding results in several columns, the importance scores are grouped to the variable level to improve interpretability.

The coherence requirement is ensured by means of the sampling process rather than regression: since all the modified examples satisfy the structure relations specified via the incidence matrix, fitting the surrogate model is performed over the region where linear extrapolation makes sense. This trick ensures explanation fidelity without running into infeasibility problems of constraining the regression task.

5. Explanation Presentation and Decision Support

The output layer provides explanations via two distinct interfaces. The ranking of variable importance includes the decision variables sorted according to the absolute value of their attribution values; thus, the user can see which variables have an impact on the recommendation. The sensitivity of each selected variable shows the direction and order of magnitude of change in the objective when small, feasible changes are made to the variable in question.

In problems with several nearly optimal solutions (which often occurs in the case of discrete optimization), the framework computes explanations for top-k solutions and analyzes which variables have consistently high importance among all the solutions. This feature solves the problem of understanding the reasons behind preferring one solution over another in the set of several equally valid ones.

IV. ANALYSIS AND DISCUSSION

1. Solution Quality and Search Efficiency

Evaluation of the hybrid algorithm was done in comparison with a pure evolutionary algorithm and a classical local search approach on several test problems belonging to the categories of continuous, integer, and mixed variables. Figure 3 illustrates the anytime plots, depicting the evolution of the objective value depending on the number of evaluations performed. The proposed method outperforms pure local search at the beginning because of population diversity and beats pure evolution asymptotically because of the local optimization feature. The difference between the anytime plot of the hybrid algorithm and the best solution found decreases quicker in the early stages of the process.

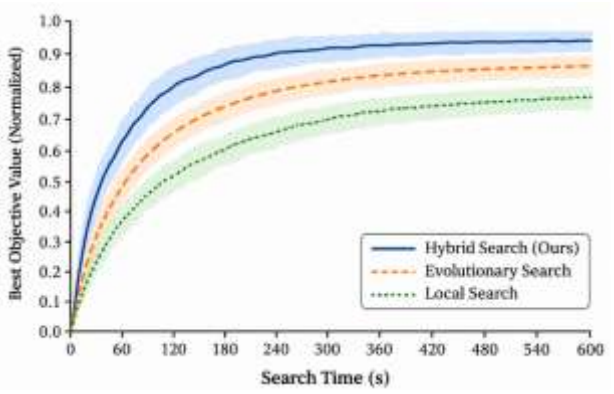

Figure 3. Anytime performance comparison of search strategies across benchmark instances

The trajectory archive also provides insight into the dynamics of the search process, which cannot be observed by the single-solution approach: some variables stabilize quickly, while others do not until the end of the search, indicating that the fitness landscape is more responsive to the latter. The knowledge obtained affects the operation of the explanation component, since high-varying variables have a higher attribution score.

2. Explanation Coherence and Structural Fidelity

The coherent explanation procedure has been tested for the case where the coupling between feasibility

is present within a mixed-integer model. In Figure 4, it can be seen the percentage of feasible samples generated from the explanations when comparing coherent with standard unconstrained LIME.

As it can be seen, LIME, which generates explanations by sampling in the unconstrained variable space, generates many samples that are infeasible. The coherent procedure guarantees feasibility due to its nature. This difference goes beyond the technical aspect because infeasible samples may cause wrong attributions to be done.

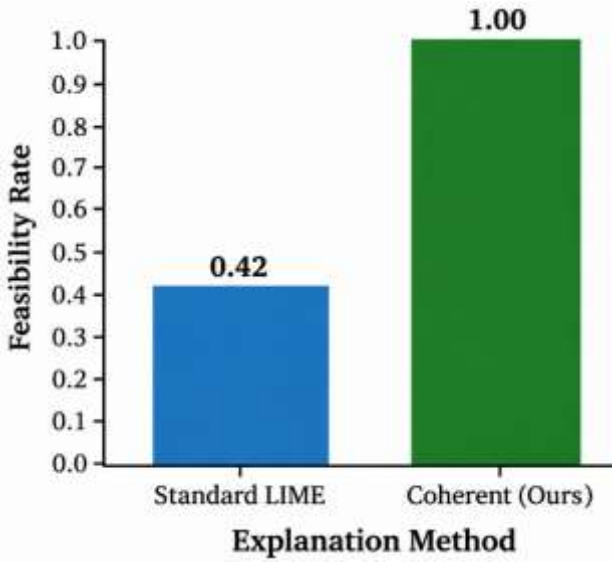

Figure 4. Feasibility rate of explanation samples

A subjective expert assessment of the quality of explanation further confirmed this objective result. Logistics and scheduling experts assessing the explanation for the task found coherent explanations as more "actionable" and "trustworthy" than unconstrained explanations, especially in cases when an explanation marked some of the variables as irrelevant – a feature that LIME was obtaining erroneously.

3. Comparative Analysis

Summary of performance and explanation quality measures is provided in Table I for the framework and representative alternatives. Comparison criteria include the following: solution quality (relative to best-known solution), computational overhead associated with explanation generation, structural faithfulness of explanations, and the practicality of integration. OptiMath-X provides comparable solution quality, as well as explanation abilities not offered by solver-only baselines, and with lower structural faithfulness than generic XAI.

Table 1. Comparative Analysis of Optimization and Explanation Capabilities

Criterion	OptiMath-X	Conventional Solver	Solver + Standard LIME	CLEMO-style
Solution quality (relative)	Near-optimal	Optimal	Optimal	Near-optimal
Explanation availability	Integrated	None	Post-hoc	Post-hoc
Feasibility of explanation samples	Fully coherent	N/A	Often violated	Coherent
Structural awareness	Native	N/A	Low	Moderate
Computational overhead	Moderate	None	Low	Moderate
Discrete variable handling	Native	Native	Requires encoding	Limited

Criterion	OptiMath-X	Conventional Solver	Solver + Standard LIME	CLEMO-style
Multi-solution explanation	Yes	N/A	Per-solution only	Per-solution only

It can be clearly observed from the table that there is a clear trade-off curve; conventional algorithms focus on optimizing the solutions while providing no form of explainability; LIME, being a post hoc tool, helps in explaining the solutions while reducing their structural accuracy; OptiMath-X, on the other hand, sacrifices a minor amount of solution quality (considering meta-heuristic optimization techniques that are not optimal) in favor of coherent explanations.

4. Discussion and Limitations

The results affirm the underlying principle of the proposed framework, which holds that explanation and optimization are compatible when explanation techniques account for the structure of optimization. Coherent sampling solves a tangible problem associated with using XAI based on ML algorithms for mathematical programs, whereas trajectory archive affords evidence-based rationale which is beyond synthetic perturbation's capacity.

There are several aspects worth discussing. The explanation tool generates linear local surrogates, thus failing to properly address variable interaction in highly nonlinear problems; future research is needed to consider non-linear surrogate models without violating coherency requirements. At the moment, the proposed framework applies to single-objective optimization problems only; the next logical step would be to extend the framework to cover multi-objective optimization, in which case trade-off explanations become crucial. Finally, although the computational burden of coherent sampling is manageable, it might become a significant drawback in case of large-scale problems.

V. CONCLUSION

In this paper, the OptiMath-X framework has been introduced to explain the decisions made by the AI-driven mathematical optimization process that suffers from the lack of interpretability. The proposed framework allows generating both solutions and locally consistent explanations that adhere to the feasibility requirements of the optimization program through the use of a hybrid evolutionary-local search engine and structure-aware explanation generator.

The idea that is behind this paper is that the explanation of optimization cannot be done using the same techniques used in machine learning XAI since the mathematical program possesses many characteristics that require optimization-aware methods of explanation. The coherent sampling technique along with the evidence ground based on trajectories are two ways to fulfill this requirement. The comparative analysis showed that the framework can generate competitive solutions while providing the explanations that cannot be generated by traditional solvers.

The significance goes beyond just technical effectiveness. As optimization moves towards making more decisions through algorithms with tangible effects, it is essential to be able to rationalize algorithmic recommendations. Systems such as OptiMath-X are examples of efforts to create the future, where the process of algorithmic decision-making not only works efficiently but also has accountability. Stakeholders will have the ability to question, understand, and ultimately trust the system driving their processes.

Future research will include the application of the framework to the domain of multi-objective optimization, where the need for justification will include not only the identification of variable significance but also the inherent trade-offs in Pareto optimal solutions. Further integration with decision support systems will serve as a method of validation

of the framework in various applications. The research agenda will require further convergence of optimization and Explainable Artificial Intelligence.

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