Careful! Training Relevance is Real

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There is a recent proliferation of research on the integration of machine learning and optimization. One expansive area within this research stream is predictive-model embedded optimization, which uses pre-trained predictive models for the objective function of an optimization problem, so that features of the predictive models become decision variables in the optimization problem. Despite a recent surge in publications in this area, one aspect of this decision-making pipeline that has been largely overlooked is training relevance, i.e., ensuring that solutions to the optimization problem should be similar to the data used to train the predictive models. In this paper, we propose constraints designed to enforce training relevance, and show through a collection of experimental results that adding the suggested constraints significantly improves the quality of solutions obtained.

Key words: Math Programming; OM Practice; Stochastic Methods

1. Introduction

The use of pre-trained predictive models in optimization decision problems is nothing new. Examples abound; consider a traditional setting in advertising. Suppose a retailer can select from among $n$ advertising channels, and fits a regression model to predict sales based on the amount of dollars allocated to each channel. Given a budget of $B$ dollars, how much should the retailer allocate to each advertising channel to maximize revenue? Classical Operations Research (OR) methods suggest that a regression model can be fit on historical data to predict revenue, and then the allocation decision variables can be selected to maximize predicted revenue. Depending on the predictive model chosen, the optimization model can be appropriately formulated. For example, if the predictive model chosen is a linear regression, the optimization problem can be modeled as a
linear programming model; if the predictive model chosen is a neural network or a random forest, recent research shows how a mixed-integer model can be formulated (for instance, Anderson et al. (2020)). We will refer to this decision-making paradigm as \textit{predictive-model embedded optimization} (PMO).

Because of its generality, PMO finds potential applications throughout the analytical landscape. There is a major issue with PMO however, which practitioners are well aware of: decisions produced by PMO are often unrealistic.

Let us demonstrate this issue using an example in a wine production context. Wine scores are typically used by critics to specify their opinion about wine quality. Suppose a wine producer is equipped with a dataset that includes physicochemical property measurements of varieties of wine as features (e.g., pH, fixed acidity, residual sugar, etc.) along with the corresponding wine scores. The producer wants to leverage this dataset and build a PMO model to determine the best combination of physicochemical property measurements that maximizes the expected wine score.

Figure 1 shows a scatter plot (pH versus fixed acidity) for two solutions obtained via a PMO model defined over a trained neural network and historical observations in the data (features are scaled between 0 and 1). The first solution is obtained by solving the corresponding optimization model without additional constraints (represented by an orange cross) and the second solution is obtained after adding our proposed constraints to enforce training relevance (represented by a blue diamond). Measurements of pH and fixed acidity in historical observations present a negative correlation, which is expected as higher acidity should correspond with a lower pH. The initial solution obtained, however, completely violates this relationship, rendering the solution unacceptable. Alternatively, the constrained solution is closer to the training data and aligns with the aforementioned chemical considerations.

The example above highlights how the solutions obtained by PMO can be inappropriate for a particular application. That is not the only potential issue. Even if a wine could be created that has the relationship of high acidity and high pH, the evaluation of the objective function at that point would be untrustworthy. If the optimization problem selects a solution far away from the training data of the predictive model, one cannot trust the prediction produced by the predictive model at that point (i.e., the error is immeasurable). This is well known in the application of predictive modeling, where it is common to assume that the unobserved/test data comes from the same distribution as the historical/training data.

Similar issues arise in the field of stochastic optimization, where a decision maker seeks to optimize the expected value of a function that depends on a random vector. Since the real distribution of the random components is unknown, the optimization model is built using an approximation of the distribution based on available data. The discrepancy between the expected objective value
of solutions obtained from these type of models and the real-world performance of said solutions has been referred to as the “optimizer’s curse” (Smith and Winkler 2006). One approach to deal with this issue is using distributionally robust optimization (Bertsimas et al. 2018, Van Parys et al. 2021) as a way to consider the worst-case performance among many potential probability distributions to approximate the real (unknown) distribution of the random vector. Another approach is using Bayesian methods (Smith and Winkler 2006, Gupta and Rusmevichientong 2021) to work with conditional expectations that can lead to better approximations of the unknown distribution.

We remark that these approaches cannot be directly translated into our PMO setting, as we are optimizing over the output of a trained predictor instead of considering an expected value, which for an empirical distribution can be simply stated as a sum of probabilities multiplied by the corresponding evaluations of the objective for the data points.

There are therefore two major issues with a vanilla application of PMO as presented thus far in this paper: (1) the solutions can be inappropriate for the application, and (2) the validity of the predictive model at the solution obtained could be untrustworthy. To address these issues, constraints can be added for each possible application to ensure that the decisions model physical or other real-world considerations, but these relationship might be highly non-linear, or perhaps unknown to the modeler. One might also try to examine all pairs of variables and make sure they are reasonably correlated as desired, but this can be challenging to identify for higher degree relationships and can lead to over constraining.

![Figure 1](image_url) A scatter plot comprising two variables (pH and fixed acidity) for two solutions from a PMO model.
We suggest a general modeling approach that addresses both issues with PMO. We investigate the use of *training relevance constraints*, which are based on the data used to train the underlying predictive model. We investigate two types of constraints, the first uses the Mahalanobis distance and is particularly useful when an assumption on multivariate normality is reasonable. The second type of constraints limits a distance measure from PMO solutions to points in the training data.

Our experimental evaluation provides clear evidence for the necessity of training relevance constraints. We first apply PMO to two global optimization benchmark problems using sampling to produce training data. We use global optimization benchmark functions because we know the optimal value, and so the quality of solutions produced with and without training relevance constraints can be measured. The results show that, independently of the predictive model used (linear regression, random forest, or neural network), the quality of the solutions are enhanced when training relevance constraints are incorporated.

These experiments also highlight an interesting observation that among the three predictive models considered, random forests are the most stable if PMO is employed without training relevance constraints. However, the incorporation of training relevance constraints nearly always leads to better solutions, even for random forests. Additionally, there are some settings where using linear regression models with training relevance constraints yields better solutions than random forests and neural networks, even if the prediction quality of the linear regression is not as good as the other models.

We then evaluate the quality of the solutions obtained by PMO on real-world data sets. Since an optimal solution is unknown, and even the quality of the solution with respect to the objective is unknown, evaluating the quality of the solutions is reduced to examining how reasonable the solutions are. We discuss both quantitative and qualitative reasons why the solutions with training relevance constraints are superior.

## 2. Literature Review

Multiple works from the literature consider optimization problems defined over trained predictive models, ranging from simple linear regressions to more complex predictive models such as random forests and neural networks. Bertsimas et al. (2016) optimize over an estimated ridge regression model seeking to improve the efficacy of chemotherapy regimens in clinical trials. Huang et al. (2019) and Baardman et al. (2019) propose optimization models defined over linear regressions in the context of retailers location decisions and scheduling of promotion vehicles, respectively. Ferreira et al. (2016) use random forests to estimate the demand of a product based on its price, and develop an optimization model over a trained random forest to determine product prices that maximize total expected revenue. Other application areas include food delivery Liu et al. (2020),
scholarship allocation Bergman et al. (2019), personalized pricing Biggs et al. (2021), and auctions Verwer et al. (2017).

Optimization problems defined over trained predictive models are often challenging to solve, depending on the properties of the underlying predictive model. Mišić (2020) and Biggs et al. (2017) propose exact solution approaches for optimization problems defined over tree ensembles. Mixed integer programming (MIP) formulations for optimization models defined over trained neural networks are studied by Cheng et al. (2017), Fischetti and Jo (2018), Bunel et al. (2018), Dutta et al. (2018), Bergman et al. (2019), Grimstad and Andersson (2019a), Schweidtman and Mitsos (2019), Tjeng et al. (2019), Grimstad and Andersson (2019b), Botoeva et al. (2020), Anderson et al. (2020) and Tsay et al. (2021). Ensembles of neural networks are studied by Wang et al. (2021). A closely related research area deals with so-called verification problems, which seek to verify relationships between the inputs and outputs of neural networks, as well as to measure the sensitivity of the outputs to small changes in the inputs. These problems are often formulated as mixed-integer programs defined over trained neural networks (Lomuscio and Maganti 2017, Cheng et al. 2017, Katz et al. 2017, Serra et al. 2018).

A related stream of literature considers data-driven stochastic optimization. In this context, the objective function depends on uncertain parameters for which the distribution is unknown, but can be estimated via a set of historical observations. Bertsimas et al. (2018) and Van Parys et al. (2021) study a robust sample average approximation (SAA) method, which considers an uncertainty set containing potential distributions for the parameters defined by a goodness-of-fit test. Gupta and Rusmevichientong (2021) proposes an improved SAA approach that estimates the parameters using Bayes’ rule and regularization techniques, leading to better performance under a small-data setting. Smith and Winkler (2006) also explores Bayesian methods to deal with the issue of the “optimizer’s curse”.

Despite the growing literature in PMO studies, the importance of training relevance seems to be overlooked by the optimization and predictive modeling community, i.e., optimal solutions found through PMOs should be similar to the training inputs. In predictive modeling, it is common to assume that the unobserved/test data comes from the same distribution as the historical/training data, which is used to build predictive models (Amodei et al. 2016), otherwise the predictive models’ applicability would be limited. Similarly, a solution obtained via PMO can be seen as a new observation in the dataset, which should only be trusted if it comes from the same distribution as the training data.

To our knowledge, Biggs et al. (2017) is the only work in the PMO literature that has considered a notion of training relevance. The authors study a property investment problem and ensure similarity between solutions found via a PMO model and the historical data by constraining the search
space to be within the convex hull of the features of historical observations. The usefulness of this approach is limited to the cases in which convex combinations of the input data points are likely to produce feasible solutions to the problem at hand. Moreover, the effect of adding these relevance constraints, in contrast to solving the unrestricted model, is not explored.

3. Training Relevance Constraints

We consider a trained predictive model that is established to learn the relationship between a dependent variable $y$ and a vector of independent variables $\mathbf{x} = \{x_1, ..., x_n\}$ based upon historical observations. We denote the predicted outcome of such a model by $F(\mathbf{x})$ and study problems of the following form:

$$\min \quad F(\mathbf{x}) \quad \text{(1a)}$$
$$\text{s.t.} \quad A\mathbf{x} \leq \mathbf{b}, \quad \text{(1b)}$$
$$1 \leq \mathbf{x} \leq \mathbf{u}, \quad \text{(1c)}$$
$$\mathbf{x} \geq 0, \quad \text{(1d)}$$

where the feasible space is given by a set of linear constraints encoded by $A \in \mathbb{R}^{m \times n}$ and $\mathbf{b} \in \mathbb{R}^m$, and vectors $\mathbf{l}, \mathbf{u} \in \mathbb{R}^n$ establish lower and upper bounds on the decision variables.

We consider three different predictive models associated with function $F(\mathbf{x})$: linear regressions, random forests, and neural networks. The mathematical formulations corresponding to each one of the three predictive models are discussed in Appendix A. In order to incorporate training relevance into model (1), we propose a class of constraints that seek to enforce a maximum distance between the decision variables vector in the optimization model and the data used to train the underlying predictive model. We propose two different ways of enforcing such a measure of distance.

3.1. Mahalanobis Distance Constraints

The Mahalanobis Distance (MD), introduced by Mahalanobis (1936), measures the number of standard deviations between a given point and the centroid of a distribution. MD has been used for detecting multivariate outliers in different application areas such as psychology (Leys et al. 2018), archaeology (Papageorgiou 2020), and geotechnics (Zheng et al. 2021).

We propose a constraint that restricts the MD between the solution vector $\mathbf{x}$ and the training data to be less than or equal to a parameter $\gamma$. Let $\Gamma(\mathbf{x})$ be the MD measure mentioned above, which is calculated as:

$$\Gamma(\mathbf{x}) = \sqrt{(\mathbf{x} - \mu)^\top C^{-1} (\mathbf{x} - \mu)}, \quad \text{(2)}$$
where $\mu$ and $C$ denote the mean vector and the covariance matrix of the training inputs, respectively. We propose adding constraint

$$\Gamma(x) \leq \gamma$$

as a way of considering training relevance in our models. We remark that for implementation purposes, the squared form of function $\Gamma$ can be directly inserted into the model and solved via off-the-shelf optimization solvers such as Gurobi (Gurobi Optimization 2020).

Parameter $\gamma$ controls the level of conservativeness of the model. Low values for $\gamma$ result in a smaller feasible region in which the solution to the optimization problem must be close to the training data. Larger values for $\gamma$ allow the outcome for the optimization model to be farther away from the training distribution. If the training inputs follow a multivariate normal distribution, then $\Gamma^2(x)$ follows a chi-square distribution with $n$ degrees of freedom, where $n$ equals the number of dimensions of the training inputs (Johnson et al. 2014). In practice, a point $\hat{x}$ is commonly labeled as a multivariate outlier if $\Gamma^2(\hat{x})$ exceeds a chi-square critical value with $n$ degrees of freedom at significance level $\alpha$ in \{0.05, 0.01, 0.001\}. As a result, if the training data follows a multivariate normal distribution, then a natural value for $\gamma$ is given by $\gamma = \sqrt{\chi_{n,1-\alpha}^2}$. We remark that in settings in which the training inputs do not follow a multivariate distribution, constraints based on MD can still be useful after tuning the value of $\gamma$.

### 3.2. K-Nearest Neighbors Constraints

Our second class of constraints considers the distance between the solution of the optimization model and the $K$ closest points from the input data, denoted as its $K$-nearest neighbors. This type of measures have been widely used for classification and regression problems (Friedman 2017). Among the multiple measures of distance available, we propose a formulation that considers the $\ell^1$-norm distance metric, which computes the sum of the absolute difference of the individual components of the vectors.

Consider a training data set $S = \{\hat{x}^1, \ldots, \hat{x}^q\}$ composed of $q$ observations $\hat{x}^j \in \mathbb{R}^n$ for $j \in \{1, \ldots, q\}$. We propose a mixed-integer linear formulation that incorporates a constraint that limits the average distance between the solution of the optimization model and its $K$-nearest neighbors to be less than or equal to a parameter $\gamma$. For all $i \in \{1, \ldots, n\}$ and $j \in \{1, \ldots, q\}$, let auxiliary decision variables $d_{ij}$ and $d_{ij}^+$ capture the deviation between the $i^{th}$ component of solution vector $x$ and the $i^{th}$ component of sample point $\hat{x}^j$. Let auxiliary decision variables $w_j$ represent the $\ell^1$ distance distance between $x$ and sample point $\hat{x}^j$. We introduce auxiliary binary decision variables $\pi_{kj}$ that take a value of 1 if sample point $\hat{x}^j$ is one of the $k^{th}$ nearest neighbors of solution vector $x$, and auxiliary variables $z_k$ to capture the $\ell^1$ distance between $x$ and the $k^{th}$ nearest point in
$S$ (for example, $z_1$ captures the distance between $x$ and the closest sample point, $z_2$ captures the distance between $x$ and the second closest sample point, and so forth). Our proposed formulation is given by

$$\begin{align*}
\min & \quad F(x) \\
\text{s.t.} & \quad Ax \leq b, \\
& \quad 1 \leq x \leq u, \\
& \quad x_i + d^+_i - d^-_i = \hat{x}_i, \quad \forall i \in \{1, \ldots, n\}, j \in \{1, \ldots, q\}, \\
& \quad w_j = \sum_{i \in \{1, \ldots, n\}} d^+_i + d^-_i, \quad \forall j \in \{1, \ldots, q\}, \\
& \quad z_k \geq w_j - M(1 - \pi_{kj}), \quad \forall j \in \{1, \ldots, q\}, k \in \{1, \ldots, K\}, \\
& \quad \sum_{j \in \{1, \ldots, q\}} \pi_{kj} = k, \quad \forall k \in \{1, \ldots, K\}, \\
& \quad \frac{1}{K} \sum_{k \in \{1, \ldots, K\}} z_k \leq \gamma, \\
& \quad \pi \in \{0, 1\}^{K \times q}, \\
& \quad x, d, w, z \geq 0.
\end{align*}$$

where $M$ is a sufficiently large constant. Constraints (4d)-(4e) define the $w$-variables, while constraints (4f)-(4g) define the $z$-variables. Note that for $k = 1$, exactly one $\pi_{1j}$ variable equals 1 and so exactly one constraint (4f) is activated, ensuring that at optimality $z_1$ equals the distance between $x$ and the closest sample point. For $k = 2$, then exactly two $\pi_{2j}$ variables take a value of 1, activating two constraints (4f). As a result, $z_2$ must be greater than or equal to two of the distances between $x$ and the sample points, captured by the $w$-variables. At optimality, $z_2$ will be exactly equal to the distance between $x$ and the second closest point in the sample. The model follows the same logic for the remaining values of $k$. Finally, constraint (4h) ensures that the average distance to the $K$-nearest neighbors is less than or equal to threshold $\gamma$.

4. Experiments

We present two sets of experimental results. Section 4.1 describes results on a set of synthetic data based on benchmark global optimization functions. Section 4.2 provides results on a real dataset. All predictive models are generated in Python using the scikit-learn package (Pedregosa et al. 2011), and all optimization models are solved with Gurobi 9.0 (Gurobi Optimization 2020) in Windows 10 on an Intel(R) Xeon(R) Gold 6130 CPU @ 2.10GHz processor with 32 GB RAM.
4.1. Experiments on Synthetic Data

We design experiments on synthetic data for solving two global optimization benchmark problems using PMO. Given a synthetic dataset generated from a global optimization benchmark function \( f(x) \), we first estimate the relationship between the independent variables (which are the decision variables in the optimization problem) and the dependent variable (which is the evaluation of the objective function) using predictive modeling, then solve the PMO model, record its solution as \( x_{PMO} \), and calculate the true objective value at the solution \( f(x_{PMO}) \). We evaluate the quality of a solution by evaluating the *optimality gap* to the true global optimal value, which is known for the benchmark function used.

4.1.1. Data Generation

We consider two benchmark functions commonly used for evaluating global optimization algorithms (Jamil and Yang 2013):

1. **Powell**: \( f(x) = (x_1 + 10x_2)^2 + 5(x_3 - x_4)^2 + (x_2 - 2x_3)^4 + 10(x_1 - x_4)^4 \). The global minimum is located at \( x^* = (0, 0, 0, 0) \), \( f(x^*) = 0 \).

2. **Quintic**: \( f(x) = \sum_{i=1}^{5} |x_i^5 - 3x_i^4 + 4x_i^3 + 2x_i^2 - 10x_i - 4| \). The global minimum is located at \( x^* = (-1, -1, -1, -1, -1) \) or \( (2, 2, 2, 2, 2) \), \( f(x^*) = 0 \).

For each function, we generate points to be used as training data for estimating the relationship between \( x \) and \( f(x) \) by sampling 1000 points from a multivariate normal distribution, with mean located at a global minimum (i.e., \( (0, 0, 0, 0) \) for Powell and \( (2, 2, 2, 2, 2) \) for Quintic) and a random covariance matrix generated using the function `make_spd_matrix` in scikit-learn. The outcome from each sampled point is the evaluation of the benchmark function, plus randomly generated noise, i.e., for point \( x \), \( y(x) = f(x) + \epsilon \). For each point, the noise is drawn from a zero-mean normal random variable with variance given by: (i) a constant \( \sigma = \delta \cdot f_{max} \), where \( \delta \) is a parameter and \( f_{max} \) is the maximum true objective value corresponding to the sampled data; and (ii) the noise terms have non-constant variance based on the true value of the function and defined as: \( \sigma(x) = \frac{1}{\beta} \cdot f(x) \), where \( \beta \) is a parameter.

We generate 10 different sets of 1000 points, each generated with a different randomly drawn covariance matrix. For each set of 1000 points, we test for \( \delta = 0.1, 0.2, \ldots, 0.6 \) and \( \beta = 2.0, 2.1, \ldots, 3.0 \). Therefore, for 2 global functions, we have 10 collections of input data, and 17 variance parameters, for a total of 340 optimization problems. We categorize the 340 problems into four scenarios, based on the function and the variance type of noise terms, i.e., Powell (constant), Powell (non-constant), Quintic (constant), and Quintic (non-constant).
Table 1  Averaged true outcomes of solutions obtained from PMO optimization models

|                  | Best Sample | Linear Regression | Random Forest | Neural Network |
|------------------|-------------|-------------------|---------------|---------------|
|                  |             | PMO  | MD  | KNN | PMO  | MD  | KNN | PMO  | MD  | KNN |
| Powell (constant) | 114         | 10721 | 1485 | 449 | 233  | 239 | 180 | 3016 | 351 | 130 |
| Powell (non-constant) | 3757      | 8905 | 3373 | 771 | 885  | 719 | 1181 | 2277 | 287 | 339 |
| Quintic (constant) | 109         | 1014 | 414  | 102 | 66   | 65  | 74  | 1344 | 103 | 72  |
| Quintic (non-constant) | 3293     | 855  | 321  | 71  | 1877 | 1933 | 593 | 2867 | 523 | 632 |
| Average           | 1818        | 5374 | 1398 | 348 | 765  | 739 | 507 | 2376 | 316 | 293 |

4.1.2. Predictive Modeling and Optimization Setup

For each dataset, we scale the independent variables to [0, 1], drop the 100 points (out of the 1,000) with highest true objective value, and randomly split the dataset into a training set and a test set in the ratio of 7 : 3. Each training set is used to fit three different predictive models: linear regression, random forest, and neural network, to be used in PMO.

For the configurations of the neurons in neural network models, we consider a structure with three hidden layers. The number of neurons in each hidden layer ranges in {1, 2, ..., 10}. For each dataset, we select the best neural network model out of 1000 candidates using the `GridSearchCV` function in `scikit-learn`. For random forest models, we create a hyper-parameters grid with the number of trees varying in {10, 20, ..., 200} and the maximum depth of the tree ranging in {1, 2, ..., 20}. We try $20 \times 20 = 400$ combinations of parameters and select the best model using `GridSearchCV`. For linear regression models, we simply fit one single model using `scikit-learn` for each dataset.

4.1.3. Optimization Results

For each predictive model fitted to each synthetic dataset, we solve three models: the vanilla PMO model (1) and two variants with our proposed training relevance constraints. For all the formulations, we define the feasible region by range constraints of the form $0 \leq x \leq 1$. For the MD constraints we set significance level $\alpha$ at 0.05, i.e., $\gamma = \sqrt{\chi^2_{n,0.05}}$. For the KNN constraints, we set $K = 1$ and $\gamma = 0.01n$. We note that the data considered for the KNN constraints is the remaining data after the removal of the 100 samples points with higher objective.

Table 1 reports the average true outcome for the solutions obtained from the optimization models over the four scenarios considered. We also report the average true value of the best solution in the sample data. The final row in the table reports the average true outcome over all the scenarios. Additional results for different values of the parameters are reported in Section B of the appendix.

We highlight several interesting observations. First and foremost, the quality of the solutions obtained through PMO are significantly better when training relevance constraints are added, independent of the predictive model chosen. Averaged over all variance settings and benchmark
functions, adding MD constraints results in solution values improving by 74%, 3%, and 87% for linear regression, random forest models, and neural networks, respectively. For \( K \)NN constraints, the solution are improved by 94%, 34%, and 88%, for the three predictive models. This is a clear indication that including training relevance constraints provides significantly better objective values. This is particularly true for linear regression and neural network models. For random forests, the use of training relevance constraints does not always improve solution quality, but it does not result in a significant reduction in solution quality either, for every setting.

Additionally, adding training relevance constraints not only improves upon the solution quality from what PMO alone provides, but it also identifies solutions that are better than the best points in the sample data. Averaged over all instances, the average objective function value of the best solution in each sample is 1818. This is reduced to 1398, 739, and 316 for MD constraints for the three predictive models, and 348, 507, and 293 for \( K \)NN constraints for the three predictive models. Without training relevance constraints, the solutions obtained through PMO are often worse than the best in sample. Hence, adding training relevance constraints allows PMO to improve on the best solution in sample, showing that the generalization of the predictive models is enhanced when solutions are constrained as suggested.

A final takeaway is that using random forests as the predictive model in PMO is best, when training relevance constraints are not considered. We hypothesize that the reason for this is that random forests never produce predictions outside of the range of \( y \) values in the training data. However, through the use of training relevance constraints, both linear regression models and neural networks can result in better solution than random forests, even when training relevance constraints are used with the random forest PMO model.

4.2. Experiments on Real Data

We now investigate the importance of training relevance on the practical feasibility of solutions for a wine quality dataset (Cortez et al. 2009), which was one of the datasets used by Mišić (2020) for investigating optimization models over random forest predictions. As done in Mišić (2020), we pre-train predictive models to predict the wine score given 11 attributes of wine. We then solve the vainilla PMO model (1) and a variant that considers \( K \)NN constraints (with \( K = 3 \)), as this variant is the best performer from the previous experiment.

The wine attributes in the dataset describe different controllable physicochemical properties, including fixed acidity, volatile acidity, citric acid, residual sugar, chlorides, free sulfur dioxide, total sulfur dioxide, density, pH, sulphates, and alcohol. We note that some of these attributes follow chemical characteristics that inherently link the variables. For example, pH and fixed acidity are negatively correlated. We evaluate the solution based on its practical feasibility. This can be
measured by whether the relationships between attributes violate chemical relationships. Since predictions from points far away from training data are untrustworthy, we can also visually inspect the proximity of the solution obtained to the training data in scatter plots.

Figure 2 plots the pairwise relationship of all 11 wine attributes for the input data points (drawn in gray circles) and the solutions obtained from the PMO models (the constrained model for random forest is omitted as the solutions are virtually the same as the ones for the unconstrained version). From the plot, we can see that it’s arbitrary as to whether a solution obeys physical properties or not without training relevance. For example, concerning pH and fixed acidity, the linear regression model finds an appropriate solution while the neural network model does not. The degree by which a solution obeys the relationship between the two variables is arbitrary if no constraints are added, but is automatically enforced through training relevance constraints. For those attributes without strong correlation we notice that the solutions obtained by the unconstrained models deviate from the distribution of the training points in general, which suggests low training relevance. In contrast, the solutions obtained from the constrained models are considerably closer to the training data.

Additionally, we note that the solutions obtained from the random forest model often fall relatively close to the training points. We hypothesize that, this is a result of random forests inherently producing results near training data since the paths in the trees are all based on splits in the training data. As with the results on the benchmark functions, this is another indication that random forests are the most reliable predictive models to be used for PMO in the absence of training relevance constraints.

5. Conclusions and Future Work

We investigate the importance of considering training relevance when solving problems modeled through PMO. We show that solutions obtained considering training relevance constraints are generally of higher quality than those obtained without training relevance constraints, using three different commonly used predictive models over benchmark functions from the global optimization literature and for a real-world data set.

There is a wide array of research that can expand on the work in this paper, including the following. First, we do not investigate specific algorithms well suited for each predictive model and type of training relevance constraint or analyze the variation in computational performance for the proposed models. Adding training relevance constraints could potentially significantly increase the solution times (e.g., consider the auxiliary binary variables and big-M constraints for the KNN setting). Advanced optimization algorithms and stronger formulations may be applicable to greatly improve computational times. Second, an investigation of which type of training relevance constraint to add for what setting is important. We show that adding training relevance constraints
nearly always leads to higher quality solutions in our experiments, but using different constraints results in varied solution quality and understanding this connection would make the decision-making pipeline more robust. Third, we only suggest two classes of training relevance constraints. There may be other ways of constraining the feasible region that are even more effective.

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Appendix

A. PMO Formulations with Different Predictive Models

A.1. Linear Regression-based PMO Formulation

\[
\min_{\mathbf{x}} \quad F(\mathbf{x}) \\
\text{s.t.} \quad \mathbf{x} \in [l, u] 
\]

(5)

\(F(\mathbf{x})\) is a linear regression model and it can be expressed as \(F(\mathbf{x}) = b_0 + b_1 x_1 + \ldots + b_n x_n\). The PMO formulation is simply a linear programming problem.

A.2. Random Forest-based PMO Formulation

A.2.1. Background of Random Forest

We consider random forest regression models in this paper, where the outcome variable \(y\) is continuous. We assume there are \(T\) trees in the random forest model and each tree \(t\) has the same weight. Each tree is built by iteratively splitting the space of training inputs \(\mathcal{D}\). After the splitting process, we have a collection of split nodes, including queries such as, “Is \(x_i \leq a\)?”, where \(a \in \mathbb{R}\). For every split node, it has two child nodes. The first split node is also called root node. After a series of splits, we arrive at a set of leaf nodes. For leaf node \(l\), it contains a portion of the \(k\) observations in \(\mathcal{D}\). The score at leaf node \(l\), \(y_{t,l}\), is the average of the outcome of the observations falling in this leaf node in tree \(t\). Given an observation with a vector of independent variables \(\mathbf{x}\), it will reach some leaf node \(l\) after checking a series of splits. Thus, the prediction of \(\mathbf{x}\) is given by \(F_t(\mathbf{x}) = y_{t,l}\). The prediction of the random forest is given by

\[
\sum_{t \in T} \frac{1}{T} F_t(\mathbf{x}) = \sum_{t \in T} \frac{1}{T} y_{t,l}
\]

A.2.2. Optimization Model

Mišić (2020) presents PMO formulations to solve optimization problems over trained random forests. Here, we adopt a slightly different formulation as it helps us to directly incorporate training relevance constraints into the optimization model. The objective of the optimization problem is to find the independent variable vector \(\mathbf{x}\) that maximizes the outcome predicted by the random forest \(F(\mathbf{x})\). Since \(F(\mathbf{x}) = \frac{1}{T} y_{t,l}\), the optimization problem is equivalent to find a leaf nodes from each tree in the random forest that maximizes the average outcome.

The random forest-based optimization problem is formulated as:

\[
\max_{\mathbf{p}, \mathbf{z}} \quad \sum_{t \in T} \sum_{l \in \text{leaves}(t)} \frac{1}{T} p_{t,l} \cdot y_{t,l} \\
\text{s.t.} \quad \sum_{l \in \text{leaves}(t)} p_{t,l} = 1, \quad \forall t \in T, 
\]

(A.1a)

(A.1b)
\[
\sum_{l \in \text{leaves}(t)} LB_{t,l} \cdot p_{t,l} \leq z_i^{LB}, \quad \forall t \in T, \forall i = 1, 2, \ldots, n, \quad (A.1c)
\]

\[
1 - \sum_{l \in \text{leaves}(t)} (1 - UB_{t,l}) \cdot p_{t,l} \geq z_i^{UB}, \quad \forall t \in T, \forall i = 1, 2, \ldots, n, \quad (A.1d)
\]

\[
z_i^{LB} \leq z_i^{UB} - \epsilon, \quad \forall i = 1, 2, \ldots, n, \quad (A.1e)
\]

\[
z_i^{LB} \in [l_i, u_i], \quad \forall i = 1, 2, \ldots, n, \quad (A.1f)
\]

\[
z_i^{UB} \in [l_i, u_i], \quad \forall i = 1, 2, \ldots, n, \quad (A.1g)
\]

\[
p_{t,l} \in \{0, 1\}, \quad \forall t \in T, \ l \in \text{leaves}(t) \quad (A.1h)
\]

We define two sets of decision variables in our model. The first set is used to determine the predicted score of tree \( t \), which is equivalent to the score of leaf node \( l \) chosen in tree \( t \). We let \( \text{leaves}(t) \) be the set of leaf nodes in tree \( t \). \( P_{t,l} \) is a binary variable, which is 1 if leaf \( l \) of tree \( t \) is chosen, 0 otherwise.

The second set of decision variables \( (z_i^{LB}, z_i^{UB}) \) is used to specify the feasible domain of each independent variable \( x_i \). We let the solution vector of \( x = (z^{LB} + z^{UB})/2 \).

The constraints have the following meaning. Constraint (A.1b) makes sure that only one leaf node can be chosen from each tree in the random forests. Since a leaf node is reached by passing a series of split nodes. Every leaf node can be connected with a series of splitting queries on the path from the root node. Therefore, each leaf node is defined by a domain \([LB_{t,l}, UB_{t,l}]\) for each variable \( x_i \). Constraint (A.1c) and constraint (A.1d) ensure that for any chosen leaf node \( l \) of tree \( t \), the domain for every independent variable \( x_i \) includes the feasible region of the same variable. Constraint (A.1e) ensures that the resulted region is not empty for \( x_i \). Constraint (A.1f) and (A.1g) enforce the resulted region of each independent variable \( x_i \) locates in its global feasible range. Constraint (A.1h) defines each \( p_{t,l} \) to be binary.

### A.3. Neural Networks-based PMO Formulation

There is plenty of literature on formulating neural networks models as a mixed integer programming problem. In particular, we make use of recent work that solve the neural networks-based optimization problem. For the details of the formulation, the reader is referred to Bergman et al. (2019).

### B. Complete Experiment Results on Synthetic Data

#### B.1. Powell (constant)

#### B.2. Powell (non-constant)
Table 2  True outcomes on data simulated using Powell function with noise having constant variance

| δ   | Best Sample | PMO | MD | 0.3 | 0.1 | 0.01 | PMO | MD | 0.3 | 0.1 | 0.01 | PMO | MD | 0.3 | 0.1 | 0.01 |
|-----|-------------|-----|----|-----|-----|------|-----|----|-----|-----|------|-----|----|-----|-----|------|
| 0.1 | 64          | 9429| 1428| 367 | 186 | 136  | 84  | 83 | 72  | 85  | 906  | 88  | 47 | 27  | 54  |
| 0.2 | 94          | 9678| 1336| 440 | 273 | 228  | 100 | 123| 112 | 146 | 159  | 2107| 113| 100 | 77  |
| 0.3 | 124         | 9801| 1139| 540 | 347 | 290  | 161 | 165| 185 | 162 | 159  | 2279| 195| 127 | 113 |
| 0.4 | 124         | 13055| 2217| 1051| 696 | 579  | 281 | 281| 264 | 277 | 188  | 4241| 145| 195 | 144 |
| 0.5 | 140         | 12450| 998 | 574 | 404 | 352  | 399 | 418| 387 | 234 | 162  | 134 | 2107| 250 | 113 | 139 |
| 0.6 | 140         | 9913 | 1791| 1204| 792 | 654  | 374 | 363| 258 | 189 | 84   | 134 | 85 | 906 | 223 |

Table 3  True outcomes on data simulated using Powell function with noise having non-constant variance

| β   | Best Sample | PMO | MD | 0.3 | 0.1 | 0.01 | PMO | MD | 0.3 | 0.1 | 0.01 | PMO | MD | 0.3 | 0.1 | 0.01 |
|-----|-------------|-----|----|-----|-----|------|-----|----|-----|-----|------|-----|----|-----|-----|------|
| 2   | 6904        | 13061| 3253| 1924| 1449| 1205 | 3575| 3767| 4140| 4807| 4926 | 3572| 246| 38  | 1699|
| 2.1 | 6904        | 12942| 3401| 2507| 1656| 1379 | 1799| 1667| 2694| 2874| 2917 | 5324| 540| 675 | 693 |
| 2.2 | 6904        | 9651 | 3270| 2754| 1942| 1673 | 2618| 1959| 3180| 3610| 3701 | 1934| 178| 1451| 1400|
| 2.3 | 6904        | 8564 | 3687| 1395| 840 | 654  | 1575| 336 | 1507| 1508| 1383 | 5117| 852| 1576| 1364|
| 2.4 | 6761        | 8905 | 3519| 844 | 552 | 461  | 165 | 165 | 165 | 165 | 165  | 1139| 170| 44  | 16  |
| 2.5 | 5091        | 5130 | 2924| 724 | 470 | 395  | 2  | 2  | 2  | 2  | 2    | 1895| 87 | 38  | 19  |
| 2.6 | 610         | 6977 | 2906| 505 | 294 | 231  | 3  | 3  | 3  | 2  | 1    | 1972| 482| 54  | 34  |
| 2.7 | 610         | 7211 | 3543| 507 | 280 | 216  | 2  | 2  | 2  | 1  | 1    | 1727| 109| 30  | 17  |
| 2.8 | 610         | 7338 | 3585| 653 | 430 | 367  | 9  | 9  | 9  | 9  | 9    | 585 | 96 | 36  | 26  |
| 2.9 | 16          | 8854 | 3666| 584 | 384 | 330  | 2  | 2  | 1  | 1  | 1    | 890 | 232| 34  | 27  |
| 3   | 16          | 9322 | 3347| 341 | 186 | 144  | 2  | 2  | 1  | 1  | 1    | 898 | 162| 27  | 11  |

B.3. Quintic (constant)

Table 4  True outcomes on data simulated using Quintic function with noise having constant variance

| δ   | Best Sample | PMO | MD | 0.3 | 0.1 | 0.01 | PMO | MD | 0.3 | 0.1 | 0.01 | PMO | MD | 0.3 | 0.1 | 0.01 |
|-----|-------------|-----|----|-----|-----|------|-----|----|-----|-----|------|-----|----|-----|-----|------|
| 0.1 | 69          | 648 | 379 | 192 | 95  | 74   | 30  | 36 | 49  | 51  | 42   | 785 | 42 | 60  | 46  | 47   |
| 0.2 | 96          | 691 | 338 | 164 | 96  | 78   | 48  | 67 | 61  | 58  | 57   | 1191| 158| 50  | 61  | 48   |
| 0.3 | 122         | 817 | 324 | 201 | 95  | 75   | 69  | 54 | 65  | 69  | 69   | 981 | 113| 58  | 56  | 52   |
| 0.4 | 122         | 935 | 471 | 220 | 116 | 92   | 60  | 56 | 72  | 73  | 72   | 1353| 94 | 85  | 70  | 68   |
| 0.5 | 122         | 1329| 421 | 242 | 107 | 82   | 79  | 93 | 117 | 83  | 83   | 1306| 72 | 103 | 91  | 66   |
| 0.6 | 122         | 1667| 553 | 210 | 101 | 84   | 110 | 84 | 116 | 113 | 111  | 2451| 140| 76  | 108 | 102  |

B.4. Quintic (non-constant)
Table 5  True outcomes on data simulated using Quintic function with noise having non-constant variance

| $\beta$ | Best Sample | Linear Regression $K$NN | Random Forest $K$NN | Neural Network $K$NN |
|--------|-------------|-------------------------|---------------------|---------------------|
|        | PMO         | MD                      | PMO    | MD   | 0.3 | 0.1 | 0.01 | PMO | MD   | 0.3 | 0.1 | 0.01 | PMO | MD   | 0.3 | 0.1 | 0.01 |
| 2      | 6730        | 935 238 202 132 131     | 5062   | 5192 | 2565 | 2507 | 2513 | 5675 | 1281 | 1952 | 1934 | 1923 |
| 2.1    | 6730        | 936 256 194 163 150     | 5062   | 4940 | 1786 | 1772 | 2196 | 3686 | 1670 | 2164 | 1478 | 1441 |
| 2.2    | 6730        | 869 285 235 166 149     | 5303   | 5152 | 1359 | 1356 | 1356 | 3027 | 185  | 533  | 508  | 501  |
| 2.3    | 6730        | 869 289 108 40 129      | 4966   | 4448 | 546  | 609  | 823  | 3818 | 667  | 1934 | 1920 | 1454 |
| 2.4    | 6357        | 826 329 110 38 127      | 35     | 1328 | 42   | 37   | 38   | 2056 | 779  | 910  | 875  | 843  |
| 2.5    | 1015        | 781 347 106 39 129      | 40     | 32   | 56   | 38   | 39   | 2694 | 283  | 126  | 33   | 32   |
| 2.6    | 936         | 781 355 83 37 37        | 45     | 40   | 41   | 45   | 44   | 3309 | 123  | 42   | 44   | 43   |
| 2.7    | 830         | 873 363 182 51 39       | 33     | 35   | 33   | 36   | 34   | 1997 | 100  | 37   | 45   | 43   |
| 2.8    | 85          | 852 362 95 40 38        | 26     | 28   | 34   | 40   | 37   | 1855 | 200  | 118  | 50   | 42   |
| 2.9    | 44          | 837 366 94 40 38        | 43     | 35   | 45   | 51   | 39   | 1694 | 232  | 43   | 37   | 37   |
| 3      | 39          | 846 345 85 39 39        | 37     | 34   | 39   | 37   | 37   | 1726 | 229  | 64   | 32   | 36   |