

A graph-structured distance for mixed-variable domains with meta variables^{*†}

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Abstract

Heterogeneous datasets emerge in various machine learning and optimization applications that feature different input sources, types or formats. Most models or methods do not natively tackle heterogeneity. Hence, such datasets are often partitioned into smaller and simpler ones, which may limit the generalizability or performance, especially if data is limited. The first main contribution of this work is a modeling framework that generalizes hierarchical, tree-structured, variable-size or conditional search frameworks. The framework models mixed-variable domains in which variables may be continuous, integer, or categorical, with some identified as meta when they influence the structure of the problem. The second main contribution is a novel distance that compares any pair of mixed-variable points that do not share the same variables, allowing to use whole heterogeneous datasets that reside in mixed-variable domains with meta variables. The contributions are illustrated on several regression experiments, in which the performance of a multilayer perceptron with respect to its hyperparameters is modeled.

Keywords. Machine learning, optimization, heterogeneous datasets, mixed-variable, meta variables, distances.

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1 Introduction

Problems that deal with heterogeneous datasets face inherent challenges that arise from several reasons, such as the generation of data from different sources, the presence of various types of variables, and data with different groups of variables. Although recent deep models, such as large language models, can natively process complicated heterogeneous objects [37], these models require massive data and computational resources to perform adequately. In practice, simpler and less costly models that do not inherently tackle heterogeneity are often employed. Hence, heterogeneous datasets are often partitioned into subsets of homogeneous data of similar types that are easier to tackle: this approach is undesirable when the amount of data is limited or *expensive-to-generate* [3, 23, 30], since the performance and generalizability can be negatively impacted.

This work has two main contributions, a comprehensive modeling framework and a novel distance function, that allow to use whole mixed-variable dataset, even if the variables vary across one data point to another. The motivation is to allow affordable models and data-driven optimization methods to handle such data heterogeneity, especially when data is limited or expensive. The work seeks to enhance models like K -nearest neighbors or Gaussian processes, and optimization methods for expensive functions, such as Bayesian optimization.

1.1 Scope of the work

In the present work, data heterogeneity is intrinsic to the problems addressed. More precisely, a dataset is generated from points of a domain \mathcal{X} that has two characteristics that implies heterogeneity: 1) it is mixed-variable, *i.e.*, a point $x \in \mathcal{X}$ is composed of finitely many variables from any type amongst categorical (cat), integer (int) or continuous (con), and 2) two points $x, y \in \mathcal{X}$ do not necessarily share the same variables and/or are not necessarily subject to same bounds. A *point* $x \in \mathcal{X}$ is arbitrary, whereas a *data point* $x_{(i)} \in \mathcal{X}$ is a point that is known and part of a dataset. The form of the dataset depends on the sort of problem, but it is always related to a domain \mathcal{X} . In supervised learning or optimization, a target function $f : \mathcal{X} \rightarrow \mathbb{R}$ is addressed with a dataset $\{(x_{(i)}, f(x_{(i)}))\}_{i=1}^N$ of $N \in \mathbb{N}$ data couples. In unsupervised learning or clustering, the dataset $\{x_{(i)}\}_{i=1}^M$ consists of $M \in \mathbb{N}$ data points.

This work primarily studies domains rather than datasets. The characteristics, properties and forms of datasets are seen as byproducts of the domains from which they are generated. Data fusion techniques that integrate multiple data subsets into a single heterogeneous dataset [16, 46], even if related, is considered out-of-the-scope for the present paper. More precisely, the modeling framework, amongst many other things, implicitly performs data fusion on subsets of data that do not share the same variables. The fusion is done by constructing the *extended domain* that considers all variables across all possible subsets. The contributions of this work can be applied to heterogeneous datasets resulting from data fusion.

In this work, the particularity that two points in a domain \mathcal{X} do not share the same variables, dimension or bounds is a consequence of the so-called *meta* variables [7]. These special variables determine if other variable(s), called *decreed*, have to be excluded or included in a point of the domain \mathcal{X} , or determine their admissible values. In addition to their variable

type, each variable is assigned a role, such as meta or decreed, that reflects either how it influences the dimension, structure or bounds of the domain \mathcal{X} , or how it is subject to the influence of other variable(s). Variables that neither influence nor are influenced by other variables are assigned the *neutral* role, and they are always included in a point. The notion of roles of variables is taken from the modeling framework introduced in [7]. These roles are further developed in the present work, notably meta-decreed variables are introduced. These variables are meta variables whose own inclusions or admissible values are determined by other meta variables. The roles of variable may be illustrated on a machine learning example in which the hyperparameters of a multilayer perceptron (MLP) must be chosen, as shown by the graph structure from Figure 1.

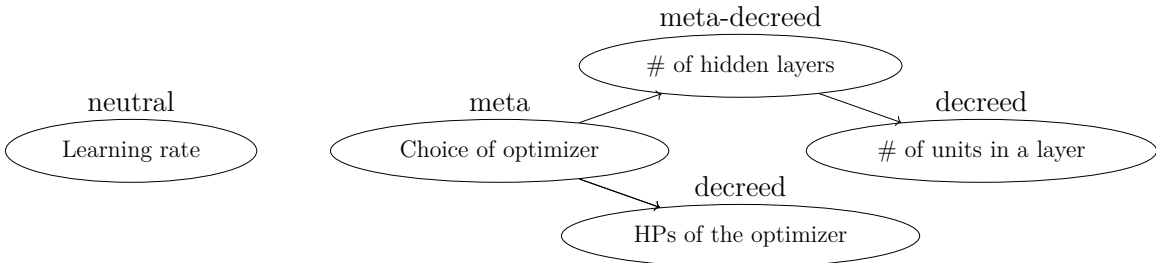


Figure 1: Graph structure for visualizing the roles of variables (hyperparameters) and the influence between hyperparameters (HPs) in the MLP example.

In the MLP example, the choice of the optimizer is a meta variable that determines the number of hidden layers that can be selected. Moreover, each optimizer has decreed variables associated to it, *e.g.*, **ADAM** is specifically associated with the running average hyperparameters. The optimizer is not a meta-decreed variable, since neither its inclusion nor its admissible values are determined by other variables. The number of hidden layers is a meta-decreed variable since its admissible values are determined by the optimizer and its value determines how many variables are present to characterize the units in the hidden layers. The variables characterizing the numbers of units are decreed but not meta as their values do not influence any other variables. The learning rate is a neutral variable since it is present in all points, and does not influence nor it is not influenced by other variables. Note that the inclusion or the admissible values of a meta-decreed variable can be determined by another meta-decreed variable: there may be several instances of meta-decreed variables. Moreover, the roles meta, meta-decreed, decreed and neutral must not be confused with the variable types, since each variable has both a type and a role.

In the MLP example, data heterogeneity emerges from two sources: 1) the diversity of variables types, *e.g.*, the optimizer that is categorical, whereas the learning rate is continuous; and 2) the meta and meta-decreed variables that determines which variables are included in point $x \in \mathcal{X}$, and the admissible values of other variable(s). The example is further detailed in Section 2.

1.2 Objectives and organization of the work

The overall objective of this work is to develop a distance function for mixed-variable domains in which two points do not necessarily share the dimension, bounds or variables.

To achieve this objective, two steps are distinguished. The first step formalizes a modeling framework that thoroughly models mixed-variable domains with meta, meta-decreed, decreed and neutral variables. The framework is based on a graph structure that encompasses all information regarding the roles of variables. In [7], meta-decreed variables are prohibited. The present work generalizes the roles of variables. In the literature, variants of graph-structured domains are referred to as tree-structured [14], hierarchical [22], variable-size [32] as well as conditional search space or neural architecture search [24]. The modeling framework generalizes and unifies all these variants.

The second step constructs a mixed-variable distance function based on the modeling framework. The distance, said graph-structured, is defined on the *extended domain* $\bar{\mathcal{X}}$, rather than directly on its corresponding domain \mathcal{X} . The extended domain is an extension of the domain that involves all included and excluded variables. Excluded variables are those that are excluded for a given point $x \in \mathcal{X}$, but present in another point $y \in \mathcal{X}$. For example, in Figure 1, the number of units in the second hidden layer is excluded, when there is only one hidden layer. Excluded variables are taken into account by the distance, since they simultaneously provide valuable information and facilitate the comparison of two points that do not share the same variables.

The rest of the document is organized as follows. First, the remainder of this section discusses related work in Section 1.3. Then, the MLP example is further developed and detailed in Section 2. Next, the extended point \bar{x} and the extended domain $\bar{\mathcal{X}}$ are thoroughly defined via the roles of variables and graph theory in Section 3. Afterwards, the graph-structured distance is defined on the extended domain $\bar{\mathcal{X}}$, which induces a distance on the original domain \mathcal{X} , in Section 4. Finally, computational experiments on the MLP example are carried out in Section 5 to compare the performance of two approaches on simple regression models. The first approach separates the regression problem into subproblems, each with homogeneous data, and the second one is based on the induced distance on the entire heterogeneous dataset.

1.3 Related work

Most literature on distances or similarity measures for heterogeneous datasets treats the simpler case where heterogeneity comes strictly from the variety of variable types. In classification, variants of K -nearest neighbors, based on distances (or similarity measures) that are built with combinations of continuous, integer or categorical distances, are commonly studied [1, 4, 33]. Decision trees or random forests are also used for classification [41], and even regression [25]. In regression, many kernel functions (similarity measures) have been recently developed for constructing Gaussian Processes (GPs) [36] over heterogeneous datasets with mixed-variable. Kernel methods are well adapted for mixed-variable problems, since mixed kernels can be directly constructed with products or additions of well-documented continuous [36], integer [19] or categorical kernels [31, 34, 39, 47].

An important reference for this work is the technical report [22], which proposes a mixed kernel function for hierarchical spaces, each paired with a directed acyclic graph (DAG), where the nodes are the variables. Variables with child nodes are required to be categorical. The kernel is constructed from one-dimensional kernels for which pseudodistances takes into account whether the variables are included or excluded. The inclusion of a variable

is managed by a designated Kronecker delta function that takes the values its ancestors as arguments. In [18], a novel similarity measure, called the earth mover’s intersection, computes similarity measures between sets of different sizes, similarly as the Jaccard index, but in a more technical fashion based on the earth mover’s distance. In [32], GPs are constructed on said variable-design spaces, which contain dimensional variables [28] that are essentially strictly discrete meta variables that determines the inclusion or exclusion of other variables. In [35], a Bayesian optimization method is used to solve deep learning structure optimization problems via graph-induced kernel functions that compute similarities between possible network architectures. The search space is modeled as a graph topology where the nodes are the architectures and the edges connect similar architectures. The kernel is based on the geodesic distance defined over nodes. In [13], feature models manage and capture heterogeneity across data points through tree-structured models consisting of features nodes and relationships arcs, that represent parent-child dependencies or integrity constraints [5]. Recent advances in features models addressed complex dependencies and constraints in large-scale heterogeneous datasets [11] with semantic logic.

This research is motivated by real-life machine learning and optimization applications. In deep learning, hyperparameter optimization is a highly studied problem in which the performance of a neural network is optimized with respect to its hyperparameters [17, 44, 45]. As mentioned previously, these mixed-variable problems includes the meta variable for the number of hidden layers that determines how many variables are present to characterize the units in the hidden layers. In [27], the optimization of a magnetic resonance device contains a variable that determines the number of magnets, and each additional heat intercept involves new design variables. In [15], an architecture design of an aircraft engine is optimized from a surrogate model constructed from a heterogeneous dataset, in which part of the data includes a fan and another part does not. More applications from various fields are also covered, including software architecture design [2], statistical medical research [21], drug discovery in heterogeneous datasets [43], multiple vehicle routing problem [20], and many more.

2 Illustration on the MLP example: domain of the hyperparameters

This section describes a working example inspired from [7] that models the domain of the hyperparameters of an MLP. The example is used to facilitate understanding of the contributions of this work and to perform computational experiments. The performance of a deep model in function of its hyperparameters can be viewed as a mixed-variable function with meta variables: let $f : \mathcal{X} \rightarrow \mathbb{R}$ be a function that outputs a performance score $f(x) \in \mathbb{R}$ for a given set of hyperparameters $x \in \mathcal{X}$, where \mathcal{X} is the domain of the hyperparameters. In practice, the performance score $f(x)$ is typically a score of accuracy on a untested data set, which is expensive-to-evaluate since the training, validation and performance test is done for a given and fixed set of hyperparameters [26].

The hyperparameters of the MLP example are presentend in Figure 2. In order to restrict the number of variables, few important hyperparameters are intentionally discarded, such as

the momentum or the batch size. The figure is composed of several tables, which are separated into different cases of optimizer variable values. The bounds of the hyperparameters $\alpha_1, \alpha_2, \alpha_3, \beta_1, \beta_2$ and β_3 are normalized for simplicity.

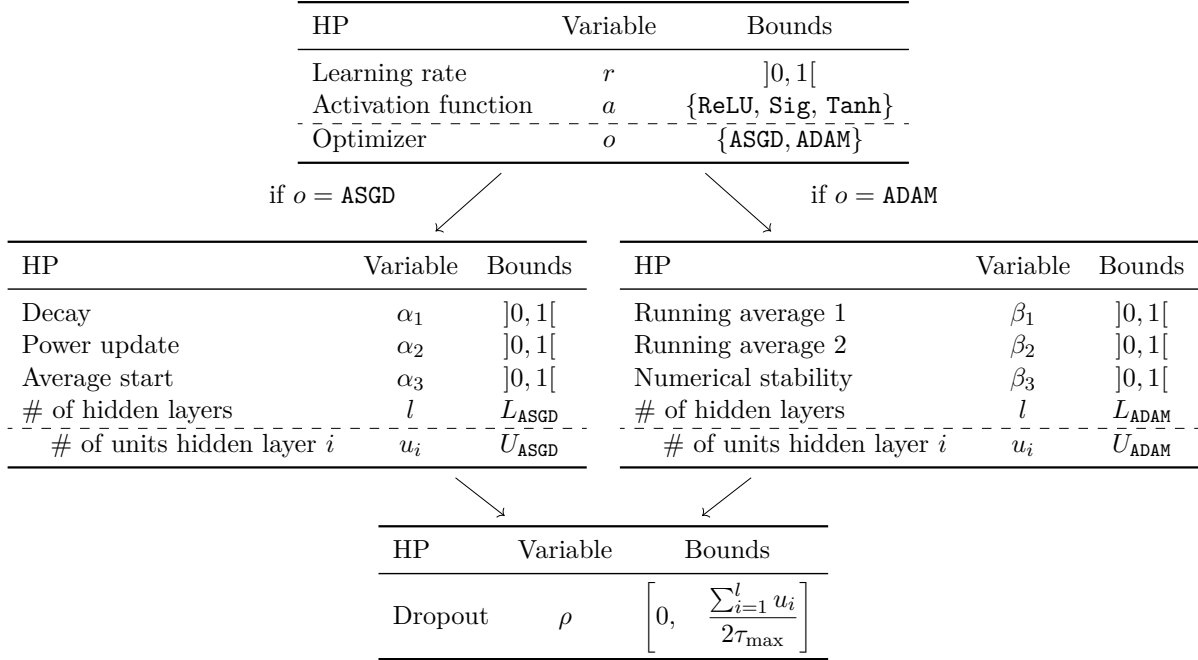


Figure 2: Hyperparameters for the MLP example.

In this work, $]a, b[$ denotes an open interval for better readability. The choice of optimizer is important. First, depending on the optimizer $o \in \{\text{ASGD, ADAM}\}$, different hyperparameters are included in a point. For example, the decay α_1 is only included if $o = \text{ASGD}$. Second, the optimizer affects the architecture. Indeed, it influences simultaneously the bounds of the number of hidden layers L_o , and the bounds U_o of every number of units $u_i \in U_o$, where $1 \leq i \leq l$. The subscript i in u_i represents the i -th hidden layer. The number of hidden layers $l \in L_o$ is influenced by the choice of the optimizer, and, most importantly, it determines the number of variables associated to the units. For example, if $l = 3$, then there are three hyperparameters u_1, u_2, u_3 for the units.

The number of hidden layers l and the number of units u_i influences the bounds of the dropout ρ , a regularization mechanism, via the following bounds dependencies

$$\rho \in \left[0, \frac{\sum_{i=1}^l u_i}{2\tau_{\max}}\right] \subseteq [0, 0.5], \quad (1)$$

where τ_{\max} is a constant that consists of the maximum sum of units that can be obtained with the hyperparameters of the MLP in Figure 2, such that

$$\tau_{\max} := \max \left\{ \sum_{i=1}^l u_i : o \in \{\text{ASGD, ADAM}\}, l \in L_o, u_i \in U_o \text{ for } 1 \leq i \leq l \right\}. \quad (2)$$

The bounds dependencies of the dropout ρ ensure that more regularization is applied to larger architectures with more units

3 Graph-structured domains

In this section, graph-structured domains that generate heterogeneous datasets are formalized. In Section 3.1, the roles of variables are explicitly introduced. Then, excluded variables and extended point, containing all variables whether they are excluded or not, are defined in Section 3.2. In Section 3.3, notions of graph theory are adapted for this work. Afterwards, the restricted sets, in which variables of the extended point belong, are detailed in Section 3.4. Subsequently, the extended domain $\overline{\mathcal{X}}$ is introduced in Section 3.5. Finally, Section 3.6 models the MLP example with the content introduced in Sections 3.1 to 3.5.

3.1 Roles of variables

The roles of variables are established from the the decree property that is generalized from [7]. The following definition allows a variable to simultaneously have the decree property, and have its inclusion or admissible values determined by a decree dependency (by other variables with the decree property): this is not allowed in [7].

Definition 1 (Decree property and decree dependency). *The decree property is attributed to variables whose values determine if other variables are included or excluded from a point $x \in \mathcal{X}$, or whose values determine the admissible values (or bounds) of other variables.*

A decree dependency refers to the inclusion or admissible values dependency of a variable with respect to an another variable with the decree property. Variables can have multiple decree dependencies with different variables.

In Section 3.3, decree dependencies are viewed as parent-children dependencies, where the values of a parent variable determines the inclusion or admissible values of its children variables. In Figure 2, the optimizer o has the decree property, since it determines the inclusion of, among others, the decay α_1 . The decay α_1 has a decree dependency with the optimizer o (parent), that is, the decay α_1 is included when $o = \text{ASGD}$, and excluded otherwise. In Section 3.4, the admissible values of a variable are determined by respecting its decree dependencies for given values of its parent variables. The number of units in the hidden layers also have the decree property, since they influence the bounds of the dropout ρ as presented in (1). The dropout ρ is always included, but its bounds are influenced by the values taken by the numbers of units and the number of hidden layers l . The dropout ρ has multiple decree dependencies, one with each number of units u_i and one with the number of hidden layers l .

Definition 1 on the decree property and decree dependency establishes four possible cases, which are formalized as the roles of variables in the following definition.

Definition 2 (Roles of variables). *The role of a variable represents its relation to the decree property. A variable is assigned one of the following roles:*

1. *meta (m), if it has the decree property, and has no decree dependency;*
2. *meta-decreed (md), if it has the decree property, and has at least one decree dependency;*

3. *decreed* (dec), if it does not have the decree property, but has at least one decree dependency;
4. *neutral* (neu), if it does not have the decree property nor decree dependency.

Recall that the role of a variable must not be confused with its variable type. Each variable has its own variable type and is assigned its own role. In the MLP example, the optimizer $o \in \{\text{ADAM}, \text{ASGD}\}$ is a categorical variable that is assigned the meta role, since it determines the inclusion and the admissible values of other variables (decree propriety), and neither its inclusion nor its admissible values are determined by other variables (no decree dependency). For convenience, a variable and its role are referred similarly as a variable and its type, *e.g.*, the optimizer is referred as a meta categorical variable. The number of hidden layers $l \in L_o$ is a meta-decreed integer variable, since its admissible values are determined by the optimizer o (decree dependency), and it determines the inclusion of the number of units u_1, u_2, \dots, u_l (decree property). The decay α_1 is a decreed continuous variable, since it does not have the decree property, and its inclusion is determined by the optimizer o . Finally, the activation function $a \in \{\text{ReLU}, \text{Sig}, \text{Tanh}\}$ is a neutral categorical variable, as it does not have the decree property, and it has no decree dependency.

3.2 Excluded variables and extended point

In [7], a point contains only variables that are included for the given values of variables with the decree property. In this work, variables that are excluded are also considered, since 1) it provides useful information for computing distances between two points of the domain \mathcal{X} that do not share the same variables, and 2) it facilitates the computations themselves. This last remark leads to the following definition.

Definition 3 (Excluded variable). *An excluded variable is a meta-decreed or decreed variable, that, for the given values of the variables associated to its decree dependencies, is not included in the given point $x \in \mathcal{X}$, but is included in at least one other point $y \in \mathcal{X}$. An excluded variable is assigned the special value **EXC** and its variable type is conserved.*

In the MLP example, the decay α_1 is a decreed continuous variable since, it is excluded when the optimizer $o = \text{ADAM}$, whereas $\alpha_1 \in]0, 1[$ (included) when $o = \text{ASGD}$. Definition 3 is introduced to allow the graph-structured distance to account every variable that is included in at least one point of the domain, collectively referred as all the included and excluded variables. The definition of an extended point formalizes the previous sentence.

Definition 4 (An extended point). *An extended point \bar{x} contains all the included and excluded variables of a corresponding point $x \in \mathcal{X}$. For $r \in R := \{\text{m}, \text{md}, \text{dec}, \text{neu}\}$ and $i \in I^r := \{1, 2, \dots, n^r\}$, the i -th variable assigned to the role r is noted \bar{x}_i^r , where $n^r \in \mathbb{N}$ is the number of variables assigned to the role r .*

The rest of this section discusses details of Definition 4. First, the bar notation is inspired by the extended set of real numbers $\bar{\mathbb{R}} = \mathbb{R} \cup \pm\{\infty\}$, referred to as the *extended real-valued* set. The notation outlines that an extended point \bar{x} is conceptually extended to incorporate

excluded variables. A point $x \in \mathcal{X}$ contains only included variables, but its variables can be attributed roles, similarly as an extended point \bar{x} .

Second, meta and neutral variables are always included, hence there is no distinction between these variables whether they are part of an extended point \bar{x} or of a point x , *i.e.*, $\bar{x}_i^r = x_i^r$ for $r \in \{\text{m, neu}\}$ and $i \in I^r$. The admissible values of meta and neutral variables are also fixed. In contrast, meta-decreed \bar{x}_i^{md} and decreed \bar{x}_j^{dec} variables of an extended point \bar{x} may be excluded from a point x , and/or their admissible values may differ between points.

Third, the framework proposed in [7] is a special case of the one developed in this work, as it includes meta variables but lacks meta-decreed variables. The special case can be recovered easily by removing the meta-decreed variables: this is convenient as the special case provides a specialized framework for problems of great interests, such as most hyperparameter optimization problems.

Fourth, decreed variables can be seen as bounds-dependent variables and, in that case, the bounds of an excluded variable are restricted to the empty set.

Finally, both the roles and types of a variables carry important information for properly computing distances between variables in Section 4. To avoid a cumbersome notation, variable types are not explicit, but they are implicitly considered in the computation of distances in Section 4. Elements of graph theory are introduced in Section 3.3. Then, further developing the variables of an extended point and their sets in Section 3.4. The extended domain $\bar{\mathcal{X}}$ is defined in Section 3.5, which allows the presentation of the graph-structured distance $\overline{\text{dist}}_p : \bar{\mathcal{X}} \times \bar{\mathcal{X}} \rightarrow \overline{\mathbb{R}}^+$ in Section 4.

3.3 Notions from graph theory

At this stage of the work, Definition 1 allows meta-decreed variables to impact each others through decree dependencies. Consequently, decree dependencies between meta-decreed variables can lead to circular reasoning or contradiction. Indeed, this can be shown with a simple example with only two meta-decreed binary variables:

$$x_1^{\text{md}} = \begin{cases} 0 & \text{if } x_2^{\text{md}} = 1, \\ 1 & \text{if } x_2^{\text{md}} = 0, \end{cases} \quad x_2^{\text{md}} = \begin{cases} 0 & \text{if } x_1^{\text{md}} = 0, \\ 1 & \text{if } x_1^{\text{md}} = 1, \end{cases}$$

where $x_1^{\text{md}} = 0 \Rightarrow x_2^{\text{md}} = 0 \Rightarrow x_1^{\text{md}} = 1 \neq 0$ (contradiction). To avoid these problematic, and uncommon situations, an assumption about the decree dependencies must be introduced. Beforehand, the role graph, which among other things allows to formulate the assumption, is defined below.

Definition 5 (Role graph). *The role graph $G = (V, A)$ is a graph structure, where*

- *V is the set of variables that contains all the included and excluded variables, represented as nodes,*
- *A is the set of decree dependencies that contains references for all inclusion-exclusion and admissible values dependencies between all the included and excluded variables, represented as arcs.*

An arc $a \in A$, which refers to a decree dependency, connects a parent (variable) to a child (variable), whose inclusion or admissible values are influenced by the parent. A parent is either a meta or meta-decreed \bar{x}_i^r , and a child is either meta-decreed or decreed, such that $a = (\bar{x}_i^r, \bar{x}_j^{r'})$, where $r \in \{m, md\}$ and $r' \in \{md, dec\}$, with $i \neq j$ when $r = r' = md$. A child can have multiple parents, and vice versa.

Now that the role graph G is properly defined, the assumption that discards situations with circular reasoning or contradiction is introduced.

Assumption 1. *The role graph G is a directed acyclic graph (DAG).*

Assumption 1 ensures that the nodes in the role graph G are (partially) ordered. Circular decree dependencies, as presented in the example with two meta-decreed variables, are forbidden. To determine such a partial order, it suffices to apply a topological sort on the role graph G .

Under Assumption 1, the role graph G is a data structure that: 1) contains all the included and excluded variables in the set of variables V , 2) contains references for all inclusion-exclusion or admissible values dependencies in the set of decree dependencies A , and 3) establishes the roles of variables according to the positions of nodes in the DAG structure:

- a meta variable \bar{x}_i^m is a root node;
- a meta-decreed variable \bar{x}_i^{md} is an internal node with at least one parent and one child;
- a decreed variable \bar{x}_i^{dec} is a leaf node with at least one parent and no child;
- a neutral variable \bar{x}_i^{neu} is an isolated node.

Recall that meta-decreed and decreed variables are child variables whose inclusions or admissible values are determined by the values of the parents that compose their decree dependencies. The role graph G outlines that the inclusion and/or admissible values of a variable can be determined by multiple different decree dependencies, that is, from multiple parents. Hence, to determine the inclusion and/or the admissible values of a variable, it is necessary to consider simultaneously all the values of its parents. In the working example, the number of units \bar{u}_i must consider simultaneously the values of its parents the optimizer \bar{o} , for its admissible values, and the number of hidden layers \bar{l} , for its inclusion. The following definition introduces formally the notion of the parents in our context.

Definition 6 (Parents). *For a given role $r \in R$ and component $i \in I^r$, the parents $\overline{\text{par}}_i^r$ of the variable \bar{x}_i^r is the subset of variables for which there exists an arc from those variables to \bar{x}_i^r , i.e.,*

$$\overline{\text{par}}_i^r := \{\bar{v} \in V : (\bar{v}, \bar{x}_i^r) \in A\}. \quad (3)$$

The parents are used to handle the inclusion-exclusion or the admissible values of meta-decreed and decreed variables in the next section. Note that although meta and neutral variables have no parents, they are still defined (as empty sets) for these roles in order to propose a concise expression for the extended domain \mathcal{X} , as in Section 3.5.

For a given variable, the inclusion or admissible values of its parents can be determined by their own parents (*i.e.*, grandparents). In Section 3.4, the ancestors of a variable, representing possible multiple generations of parents and grandparents, will be used to determine all the values that such variable can take across all possible extended points. In the MLP example, the bounds of the dropout ρ , as expressed in (1), justifies the need for ancestors. In fact, the admissible values (the bounds) of the dropout ρ are determined by the given values of its parents the number of hidden layers l and the number of units u_i . However, the constant τ_{\max} in (2), which influences all the possible values of the dropout ρ , is determined by also considering the optimizer o (grandparent). Note that the bounds of the dropout ρ do not have an explicit dependency with the values of the optimizer o since, for a given MLP problem, the constant τ_{\max} is fixed. The ancestors can be defined recursively by starting at the parents, then passing by the parents of the parents, and so on, until the roots are reached.

Definition 7 (Ancestors). *For $r \in R$ and $i \in I^r$, the ancestors of the variable \bar{x}_i^r , noted $\overline{\text{anc}}_i^r$, is the subset of variables that are either parents or recursively ancestors of parents of \bar{x}_i^r , *i.e.*,*

$$\overline{\text{anc}}_i^r := \overline{\text{par}}_i^r \cup \left(\bigcup_{\bar{x}_j^{r'} \in \overline{\text{par}}_i^r} \overline{\text{anc}}_j^{r'} \right) \quad (4)$$

where $\overline{\text{anc}}_j^{r'}$ denotes the ancestors of the parent variable $\bar{x}_j^{r'}$. The recursion in (4) stops at the root nodes, *i.e.*, with $\overline{\text{par}}_j^m = \emptyset, \forall j \in I^m$.

Now that several notions of graph theory have been adapted to this work, the definition of a graph-structured domain is formally established.

Definition 8 (Graph-structured domain). *A graph-structured domain is a domain with at least one variable with the decree property, *i.e.*, at least one meta variable.*

Definition 8 is one specific approach to formalize a graph-structured domain, yet there exist several equivalent statements.

Theorem 1 (Graph-structured domain equivalences). *Let $\mathcal{X} \neq \emptyset$, with $G = (V, A)$ as its corresponding role graph. Then the following statements are equivalent:*

1. \mathcal{X} is a graph-structured domain.
2. The set of decree dependencies is non-empty, *i.e.* $A \neq \emptyset$.
3. There is a least one point containing a variable with a least one parent.

Proof. The theorem is a direct consequence of Definitions 5 and 7. □

Theorem 1 emphasizes that the different bounds or inclusion-exclusion of variables within a graph-structured domain \mathcal{X} is a consequence of interrelationships between variables, that is, its decree dependencies (see Definition 1). Note that a variable with missing entries can be modeled as a decreed variable whose inclusion is determined by an additional binary meta variable.

3.4 Universal sets and restricted sets

As mentioned in Section 3.3, meta-decreed and decreed variables are subjected to the values of their parents, since they must respect their decree dependencies for the given values of their parents. In this section, the dependencies of a variable with respect to its parents are modeled through its restricted set, that is obtained by conditioning its universal set with the values of its parents. The universal set is defined next.

Definition 9 (Universal set). *For $r \in R$ and $i \in I^r$, the universal set $\overline{\mathcal{X}}_i^r$ of the variable \overline{x}_i^r is the set that contains all possible values that the variable can take by considering all possible values assigned to its ancestors $\overline{\text{anc}}_i^r$.*

In the example, the universal set of the number of units \overline{u}_i is $\overline{U} = U_{\text{ASGD}} \cup U_{\text{ADAM}} \cup \{\text{EXC}\}$. The number of units \overline{u}_i can be excluded, depending on the number of hidden layers \overline{l} , hence its universal set must contain the special value **EXC**.

As discussed in the previous section, the values of the ancestors must be considered, in addition to those of the parents, to determine a universal set. In the MLP example, the universal set of the dropout ρ reduces to $\overline{P} = [0, 0.5]$, *i.e.*, it is obtained when $\sum_{i=1}^l u_i = \tau_{\max}$. Recall that, from (1), the bounds of the dropout ρ depends on its parents the number of hidden layers l and the number of units u_i . However, to determine its universal set \overline{P} , the constant $\tau_{\max} = \max \{ \sum_{i=1}^l u_i : o \in \{\text{ASGD}, \text{ADAM}\}, l \in L_o, u_i \in U_o \text{ for } 1 \leq i \leq l \}$ must be determined by considering the optimizer o (grandparent). Again, τ is a constant, hence the dropout ρ has no decree dependency with the optimizer o .

The next step is to develop the restricted set of a variable. The restricted set of the variable \overline{x}_i^r is the subset of the universal set $\overline{\mathcal{X}}_i^r$ such that \overline{x}_i^r respects the decree dependencies for the given values of its parents $\overline{\text{par}}_i^r$, which are identified by arcs of the role graph G . The formal definition of the restricted set is presented below.

Definition 10 (Restricted set). *For $r \in R$ and $i \in I^r$, the restricted set of the variable \overline{x}_i^r is the universal set $\overline{\mathcal{X}}_i^r$ conditioned by the values of its parents $\overline{\text{par}}_i^r$, expressed as*

$$\overline{\mathcal{X}}_i^r / \overline{\text{par}}_i^r := \{ \overline{x}_i^r \in \overline{\mathcal{X}}_i^r : \forall (\overline{v}, \overline{x}_i^r) \in A, \overline{x}_i^r \text{ respects the decree dependencies for the values of } \overline{v} \}.$$

Meta and neutral variables are always included and have no parent, hence their restricted set is simply their universal set: $\overline{\mathcal{X}}_i^{\text{m}} / \overline{\text{par}}_i^{\text{m}} = \overline{\mathcal{X}}_i^{\text{m}} \forall i \in I^{\text{m}}$ and $\overline{\mathcal{X}}_j^{\text{neu}} / \overline{\text{par}}_j^{\text{neu}} = \overline{\mathcal{X}}_j^{\text{neu}} \forall j \in I^{\text{neu}}$. The restricted set of a meta-decreed or decreed variable requires the values of its parents for determining both its inclusion and its admissible values when it is included. If the decree dependencies, given the values of parent variables, dictate that a child is excluded, then its restricted set is **{EXC}**. In the MLP example, the restrictive set of $\overline{\alpha}_1$ is **{EXC}** when the optimizer $\overline{o} = \text{ADAM}$. The notation $/\overline{\text{par}}_i^r$ for a restricted set $\overline{\mathcal{X}}_i^r / \overline{\text{par}}_i^r$ means “*given*” the values of its parents. The parents are placed as subscripts to outline the dependency.

3.5 Extended domain and transfer mapping

Now that the restricted sets have been detailed, the extended domain $\overline{\mathcal{X}}$ is formally introduced.

Definition 11 (Extended domain). *The extended domain $\overline{\mathcal{X}}$ is a graph-structured domain constructed from a domain \mathcal{X} , its corresponding role graph $G = (V, A)$ and from the restricted sets of all included and excluded variables. The extended domain $\overline{\mathcal{X}}$ is expressed as*

$$\overline{\mathcal{X}} := \{ \overline{x} : \overline{x}_i^r \in \overline{\mathcal{X}}_i^r / \overline{\text{par}}_i^r, \forall r \in R, \forall i \in I^r \}.$$

Definition 11 expresses that an extended point $\overline{x} \in \overline{\mathcal{X}}$ must respect all the inclusion-exclusion or admissible values dependencies, *i.e.*, decree dependencies, between its variables. Recall that the main objective is to equip the domain \mathcal{X} with a distance $\text{dist}_p : \mathcal{X} \times \mathcal{X} \rightarrow \overline{\mathbb{R}}^+$ to facilitate optimization or machine learning tasks on domains that involve heterogeneous dataset. This will be done by introducing the graph-structured distance $\overline{\text{dist}}_p : \overline{\mathcal{X}} \times \overline{\mathcal{X}} \rightarrow \overline{\mathbb{R}}^+$ on the extended domain $\overline{\mathcal{X}}$, and then by inducing a distance on the domain via the bijective mapping defined in the following theorem.

Theorem 2 (One-to-one correspondence). *The transfer mapping $T_G : \mathcal{X} \rightarrow \overline{\mathcal{X}}$, which assigns the extended point $T_G(x) \in \overline{\mathcal{X}}$ to any point $x \in \mathcal{X}$ by adding its excluded variables determined by the role graph G , is a bijection.*

Proof. Injectivity. Let $x, y \in \mathcal{X}$ be such that $x \neq y$. By definition of T_G , there is a least one variable whose value differ between the two extended points $\overline{x} = T_G(x)$ and $\overline{y} = T_G(y)$, since 1) there is a least one included variable between x and y that does not share the same value; or 2) there is a least one variable that is strictly excluded for one point between x and y . Therefore, there is a least one variable that also does not share the same value in the extended points \overline{x} and \overline{y} . This show that T_G is injective since $x \neq y \Rightarrow T_G(x) \neq T_G(y)$.

Surjectivity. Let $\overline{x} \in \overline{\mathcal{X}}$ be an extended point. Then, let $G' = (V', E')$ be the subgraph of the role graph G obtained by removing the nodes and arcs corresponding to the excluded variables that take the value EXC in \overline{x} . The set V' is nonempty since either \overline{x} has no meta variables and thus $V' = V$, or \overline{x} has at least one meta variable $\overline{x}_i^m = x_i^m \in V'$. Thus, V' is the set of variables that are included in \overline{x} , and E' is the set of decree dependencies between the included variables of \overline{x} . By construction, each variable in V' respects the decree dependencies between the other variables in the set V' . Let x be the point that contains only the included variables of the extended point \overline{x} , *i.e.*, the variables in the set V' . The point x necessarily belongs to domain \mathcal{X} , since it only contains included variables that respect the decree dependencies between each others. Indeed, otherwise, if the decree dependencies would not be respected, then x would 1) contain a variable that should not be included; or 2) not contain a variable that should be included; or 3) contain an included variable that would take a value that is not allowed by the decree dependencies. Then, by definition of the mapping T_G , $T_G(x) = \overline{x}$, since $x \in \mathcal{X}$ contains all the included variables of the extended point $\overline{x} \in \overline{\mathcal{X}}$. This shows that T_G is thus surjective, since $\forall \overline{x} \in \overline{\mathcal{X}}, \exists x \in \mathcal{X}$, such that $T_G(x) = \overline{x}$.

The transfer mapping T_G is both injective and surjective, thus bijective. \square

A consequence of Theorem 2 is that if a distance $\overline{\text{dist}}_p : \overline{\mathcal{X}} \times \overline{\mathcal{X}} \rightarrow \overline{\mathbb{R}}^+$ is well-defined on the extended domain $\overline{\mathcal{X}}$, then a distance $\text{dist}_p : \mathcal{X} \times \mathcal{X} \rightarrow \overline{\mathbb{R}}^+$ can be induced on the domain \mathcal{X} with the bijective transfer mapping $T_G : \mathcal{X} \rightarrow \overline{\mathcal{X}}$. This is done in Section 4.

3.6 Illustration on the MLP example: graph-structured domain

Section 3 introduced many definitions and mathematical expressions. To facilitate the comprehension, the MLP example is modeled in this section. Before developing the role graph, the preliminary step is to model each variable and its set, which takes into account its decree dependencies, for a point $x \in \mathcal{X}$. Variables are modeled by following the decree dependencies, starting with the meta and neutral variables, then modeling variables with decree dependencies whose determining variables have been previously modeled.

The first variables to be modeled are the optimizer $o \in \{\text{ASGD}, \text{ADAM}\}$, the learning rate $r \in]0, 1[$, and the activation function $a \in \{\text{ReLU}, \text{Sig}, \text{Tanh}\}$. Next, meta-decreed and decreed variables whose decree dependencies involve only meta variables are modeled. The variables α_1, α_2 and α_3 are included if and only if $o = \text{ASGD}$, and the variables β_1, β_2 and β_3 are included if and only if $o = \text{ADAM}$. The number l of hidden layers is constrained to a set that depends on the optimizer o :

$$l \in L_o = \begin{cases} L_{\text{ASGD}} = \{0, 1, 2, 3\} & \text{if } o = \text{ASGD}, \\ L_{\text{ADAM}} = \{0, 1, 2, 3, 4\} & \text{if } o = \text{ADAM}. \end{cases}$$

The number of units u_i is included if $1 \leq i \leq l \leq l_{\max} = 4$ and its bounds depends on the optimizer o :

$$u_i \in U_o = \begin{cases} U_{\text{ASGD}} & \text{if } o = \text{ASGD}, \\ U_{\text{ADAM}} & \text{if } o = \text{ADAM}. \end{cases}$$

There are at most four unit variables in the architecture. Finally, the dropout ρ is always included, but its bounds depends on the number of the hidden layers l and the number of units u_1, u_2, \dots, u_l as expressed in (1).

The next modeling step is to build the role graph $G = (V, A)$. The set of nodes correspond to all included and excluded variables $V = \{\bar{o}, \bar{\alpha}_1, \bar{\alpha}_2, \bar{\alpha}_3, \bar{\beta}_1, \bar{\beta}_2, \bar{\beta}_3, \bar{l}, \bar{u}_1, \bar{u}_2, \bar{u}_3, \bar{u}_4, \bar{\rho}, \bar{r}, \bar{a}\}$. The arcs A of the graph represent pairs of parent-child variables, in which the child has a decree dependency with its parent. For example, the number of hidden layers l and the number of units u_i are all parents of the dropout ρ , since they determine its bounds. The role graph $G = (V, A)$ of the MLP example is illustrated in Figure 3. The role graph G schematically models a great deal of information, including 1) all included and excluded variables, 2) the role of each variable via their node position, 3) the dependencies of the restricted sets of meta-decreed and decreed variables with their parents.

The third modeling step is to determine the universal sets of meta-decreed and decreed variables. The universal sets of meta and neutral variables are directly given by the problem statement. The universal set of the number of hidden layers \bar{l} , the dropout ρ , and the number of units \bar{u}_i are respectively $\bar{L} = L_{\text{ASGD}} \cup L_{\text{ADAM}}$, $\bar{P} = [0, 0.5]$, and $\bar{U}_i = U_{\text{ASGD}} \cup U_{\text{ADAM}} \cup \{\text{EXC}\}$ for $1 \leq i \leq l_{\max}$.

Afterwards, the fourth modeling step is to express the restricted sets $\bar{\mathcal{X}}_i^r / \bar{\text{par}}_i^r$. The restricted sets of meta and neutral variables are identical to their universal set $\bar{\mathcal{X}}_i^r$, which can be expressed as

$$\bar{x}_1^m = \bar{o} \in \{\text{ASGD}, \text{ADAM}\}, \quad \text{and} \quad (\bar{x}_1^{\text{neu}}, \bar{x}_2^{\text{neu}}) = (\bar{r}, \bar{a}) \in]0, 1[\times \{\text{ReLU}, \text{Sig}, \text{Tanh}\}.$$

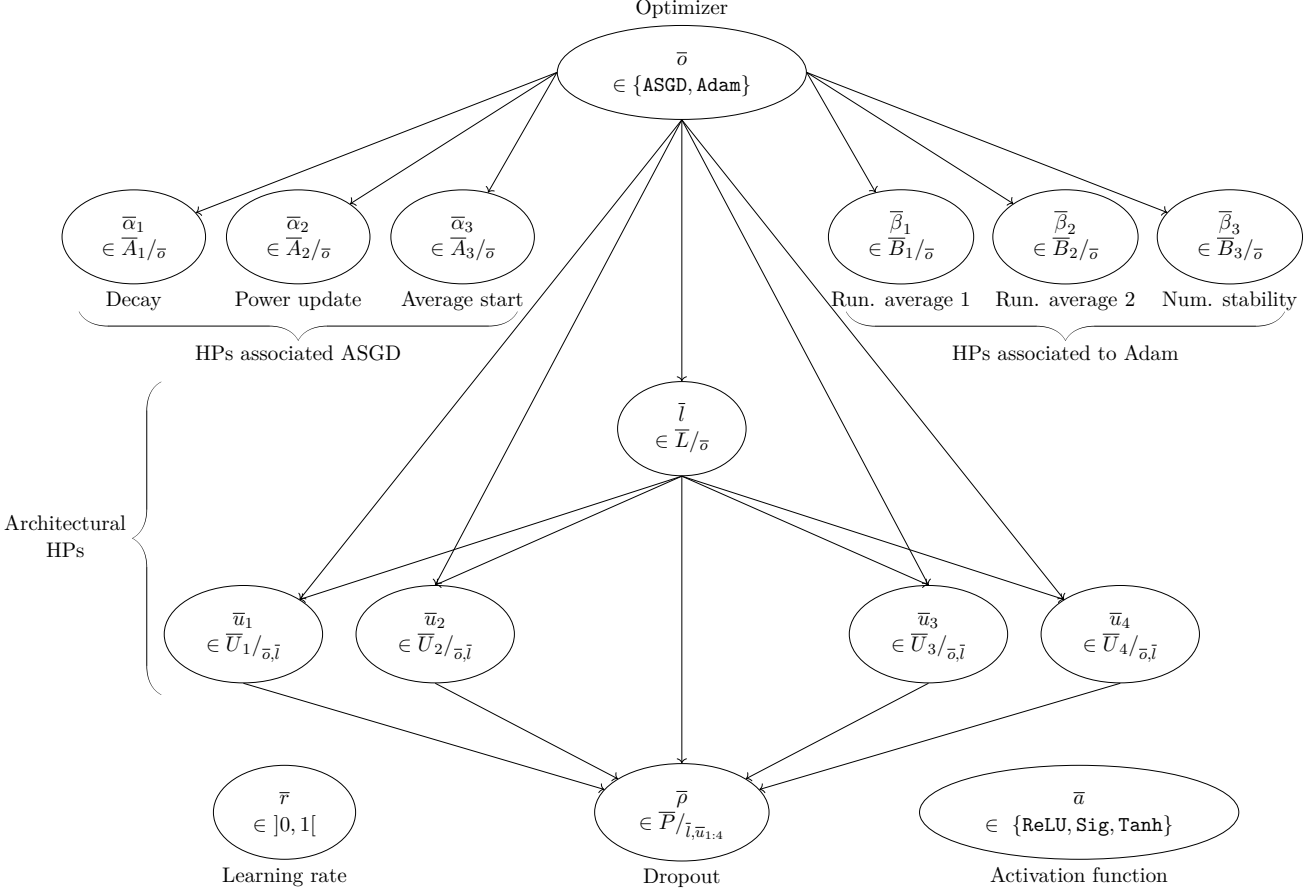


Figure 3: Role graph G for the MLP example.

Meta-decreed variables and their restricted sets are expressed as

$$(\bar{x}_1^{\text{md}}, \bar{x}_2^{\text{md}}, \bar{x}_3^{\text{md}}, \bar{x}_4^{\text{md}}, \bar{x}_5^{\text{md}}) = (\bar{l}, \bar{u}_{1:4}) \in \bar{L}/\bar{\alpha} \times \prod_{i=1}^4 \bar{U}_i/\bar{\alpha}, \bar{l}$$

where $\bar{u}_{1:4} := (\bar{u}_1, \bar{u}_2, \bar{u}_3, \bar{u}_4)$, and

$$\bar{L}/\bar{\alpha} = \begin{cases} L_{\text{ASGD}} & \text{if } \bar{\alpha} = \text{ASGD}, \\ L_{\text{ADAM}} & \text{if } \bar{\alpha} = \text{ADAM}, \end{cases} \quad \text{and} \quad \bar{U}_i/\bar{\alpha}, \bar{l} = \begin{cases} U_{\text{ASGD}} & \text{if } \bar{\alpha} = \text{ASGD} \text{ and } 1 \leq i \leq \bar{l}, \\ U_{\text{ADAM}} & \text{if } \bar{\alpha} = \text{ADAM} \text{ and } 1 \leq i \leq \bar{l}, \\ \{\text{EXC}\} & \text{otherwise,} \end{cases}$$

with $1 \leq i \leq \bar{l}$. Decreed variables are expressed as

$$(\bar{x}_1^{\text{dec}}, \bar{x}_2^{\text{dec}}, \bar{x}_3^{\text{dec}}, \bar{x}_4^{\text{dec}}, \bar{x}_5^{\text{dec}}, \bar{x}_6^{\text{dec}}, \bar{x}_7^{\text{dec}}) = (\bar{\alpha}_{1:3}, \bar{\beta}_{1:3}, \bar{\rho}) \in \prod_{i=1}^3 \bar{A}_i/\bar{\alpha} \times \prod_{j=1}^3 \bar{B}_j/\bar{\alpha} \times \bar{P}/\bar{l}, \bar{u}_{1:4},$$

where $\bar{\alpha}_{1:3} := (\bar{\alpha}_1, \bar{\alpha}_2, \bar{\alpha}_3)$, $\bar{\beta}_{1:3} := (\bar{\beta}_1, \bar{\beta}_2, \bar{\beta}_3)$, and

$$\bar{A}_i/\bar{\alpha} = \begin{cases}]0, 1[& \text{if } \bar{\alpha} = \text{ASGD}, \\ \{\text{EXC}\} & \text{if } \bar{\alpha} = \text{ADAM}, \end{cases} \quad \text{and} \quad \bar{B}_j/\bar{\alpha} = \begin{cases} \{\text{EXC}\} & \text{if } \bar{\alpha} = \text{ASGD}, \\]0, 1[& \text{if } \bar{\alpha} = \text{ADAM}, \end{cases}$$

with $i, j \in \{1, 2, 3\}$, and

$$\bar{P}/_{\bar{l}, \bar{u}_{1:4}} = \left[0, \frac{\sum_{i=1}^{\bar{l}} \bar{u}_i}{2\tau_{\max}} \right] \subseteq [0, 0.5]. \quad (5)$$

Finally, the extended domain $\bar{\mathcal{X}}$ is constructed with the restricted sets as follows

$$\bar{\mathcal{X}} = \left\{ \begin{array}{ll} \bar{x} & : \quad \bar{o} \in \{\text{ASGD}, \text{ADAM}\}, \\ (\bar{l}, \bar{u}_{1:4}) & \in \bar{L}/_{\bar{o}} \times \prod_{i=1}^4 \bar{U}_i/_{\bar{o}, \bar{l}}, \\ (\bar{\alpha}_{1:3}, \bar{\beta}_{1:3}, \bar{\rho}) & \in \prod_{i=1}^3 \bar{A}_i/_{\bar{o}} \times \prod_{j=1}^3 \bar{B}_j/_{\bar{o}} \times \bar{P}/_{\bar{l}, \bar{u}_{1:4}}, \\ (\bar{r}, \bar{a}) & \in]0, 1[\times \{\text{ReLU}, \text{Sig}, \text{Tanh}\} \end{array} \right\}.$$

4 Distance for graph-structured domains

In this section, the graph-structured distance $\overline{\text{dist}}_p : \bar{\mathcal{X}} \times \bar{\mathcal{X}} \rightarrow \bar{\mathbb{R}}^+$ is defined. Section 4.1 presents the included-excluded distance function that can compute distances for variables that can be included or excluded. The included-excluded distances of the MLP example are modeled in Section 4.2. Finally, Section 4.3 presents the graph-structured distance that is constructed with included-excluded distances, one per variable.

4.1 Included-excluded distances

For two extended points $\bar{x}, \bar{y} \in \bar{\mathcal{X}}$, the distance regarding the i -th variable assigned to role r , respectively \bar{x}_i^r and \bar{y}_i^r , is computed through three cases:

1. both \bar{x}_i^r and \bar{y}_i^r are excluded, hence the distance is set to zero;
2. exactly one variable \bar{x}_i^r or \bar{y}_i^r is excluded, hence the distance is set to a parameter that models a distance between a variable that is included for one extended point, and excluded for the other extended point;
3. both \bar{x}_i^r and \bar{y}_i^r are included, hence an one-dimensional distance function d is used, *e.g.*, the Euclidean distance [42].

Recall that a meta or neutral variable $\bar{x}_i^r \in \bar{\mathcal{X}}_i^r$ is always included, hence for $r \in \{\text{m}, \text{neu}\}$, the distance between \bar{x}_i^r and \bar{y}_i^r is always computed in the third case. For a meta-decreed or decreed variable, the restricted sets of \bar{x}_i^r and \bar{y}_i^r may differ, hence its corresponding included-excluded distance must be defined on its universal set $\bar{\mathcal{X}}_i^r$ in order to allow comparisons of any pairs \bar{x}_i^r, \bar{y}_i^r with different restricted sets. In the MLP example, the universal set of the number of units \bar{u}_i is $\bar{U} = U_{\text{ASGD}} \cup U_{\text{ADAM}} \cup \{\text{EXC}\}$. Hence, to compare the number of units \bar{u}_i from any two pairs of extended points, the corresponding included-excluded distance of \bar{u}_i must be defined on its universal set \bar{U} . The following theorem formalizes the discussion above on the three cases and the universal set by introducing a novel distance based on distances proposed in [40, 38].

Theorem 3 (Included-excluded distance). Let $\overline{\mathcal{X}}_i^r$ be the universal set of the i -th variable assigned to the role $r \in R$, noted \overline{x}_i^r , and define $\overline{\mathcal{Y}}_i^r = \overline{\mathcal{X}}_i^r \setminus \{\text{EXC}\}$. Consider $d : \overline{\mathcal{Y}}_i^r \times \overline{\mathcal{Y}}_i^r \rightarrow \overline{\mathbb{R}}^+$, a one-dimensional extended real-valued distance for the variable \overline{x}_i^r when it is included, and $\theta_i^r \in \overline{\mathbb{R}}^+$ a parameter greater than or equal to $\sup\{d(\mu, \nu) : \mu, \nu \in \overline{\mathcal{Y}}_i^r\}/2$. Then, for $u, v \in \overline{\mathcal{X}}_i^r$, the function $d_i^r : \overline{\mathcal{X}}_i^r \times \overline{\mathcal{X}}_i^r \rightarrow \overline{\mathbb{R}}^+$ defined by

$$d_i^r(u, v) := \begin{cases} d(u, v) & \text{if } u \neq \text{EXC} \neq v \text{ (both included),} \\ 0 & \text{if } u = \text{EXC} = v \text{ (both excluded),} \\ \theta_i^r & \text{otherwise (one excluded),} \end{cases} \quad (6)$$

is a one-dimensional extended real-valued distance function.

Proof. Let $r \in R$ and $i \in I^r$. The identity of indiscernibles, nonnegativity and symmetry of d_i^r are trivially proven since θ_i^r is strictly positive and since d is a distance function. The rest of the proof consists of proving that d_i^r satisfies the triangle inequality. Let $u, v, z \in \overline{\mathcal{X}}_i^r$:

Case 1 (both variables are excluded): if $u = \text{EXC} = v$, then

$$d_i^r(u, v) = 0 \leq d_i^r(u, z) + d_i^r(z, v), \text{ by nonnegativity of } d_i^r.$$

Case 2 (only one variable is excluded, by symmetry v): if $u \neq \text{EXC} = v$ and

- if $z \neq \text{EXC}$, then

$$d_i^r(u, v) = \theta_i^r \leq d(u, z) + \theta_i^r = d_i^r(u, z) + d_i^r(z, v), \text{ by nonnegativity of } d.$$

- if $z = \text{EXC}$, then

$$d_i^r(u, v) = \theta_i^r \leq \theta_i^r + 0 = d_i^r(u, z) + d_i^r(z, v).$$

Case 3 (both variables are included): if $u \neq \text{EXC}$ and $v \neq \text{EXC}$ and

- if $z \neq \text{EXC}$, then

$$d_i^r(u, v) = d(u, v) \leq d(u, z) + d(z, v) = d_i^r(u, z) + d_i^r(z, v).$$

- if $z = \text{EXC}$, then

$$d_i^r(u, v) = d(u, v) \leq \sup\{d(\mu, \nu) : \mu, \nu \in \overline{\mathcal{Y}}_i^r\} \leq 2\theta_i^r = d_i^r(u, z) + d_i^r(z, v).$$

□

Multiple comments on Theorem 3 that introduces the included-excluded distance are provided.

First, the included-excluded distance is precisely useful for meta-decreed and decreed variables that can have different restricted sets, *i.e.* that can be included or excluded,

and/or have different admissible values. As mentioned previously, for variables that are always included, such as meta and neutral variables, included-excluded distances are always computed with the both included case. The included-excluded distance is nevertheless defined for these variables in order to obtain a concise formulation of the graph-structured distance in Section 4.3.

Second, the included-excluded distance is compatible with any variable type. Indeed, in (6), the two cases both excluded and one excluded does not regard the variable type, and the case both included allows to use any distance function d .

Third, the universal set $\overline{\mathcal{X}}_i^r$ allows to compare any pair of variables $\overline{x}_i^r, \overline{y}_i^r$. Moreover, it is also necessary to establish a lower bound on the parameter θ_i^r , which ensures the triangular inequality in the last case of the proof. The inequality $\theta_i^r \geq \sup\{d(\mu, \nu) : \mu, \nu \in \overline{\mathcal{X}}_i^r \setminus \{\text{EXC}\}\}/2$ implies that the distance $d_i^r(\overline{x}_i^r, \overline{y}_i^r) = \theta_i^r$ (one excluded case) must be at least half the largest distance between any pairs of included variables $\overline{x}_i^r, \overline{y}_i^r$, with possibly different restricted sets. In the MLP example, recall that the universal set of the number of units \overline{u}_i is $\overline{U} = U_{\text{ASGD}} \cup U_{\text{ADAM}} \cup \{\text{EXC}\}$. Therefore, the parameter θ_i^r for \overline{u}_i must be greater than $(\max(\overline{U}') - \min(\overline{U}'))/2$, where $\overline{U}' = U_{\text{ASGD}} \cup U_{\text{ADAM}}$. Apart from its lower bound, the parameter θ_i^r is flexible.

Fourth, the included-excluded distance is more formally an extended real-valued one [12], since it is allowed to take the infinite value. The infinity value allows to consider meta-decreed or decreed variables with unbounded restricted sets. For example, let $r \in \{\text{md}, \text{dec}\}$ and $i \in I^r$, such that $\overline{\mathcal{X}}_i^r / \overline{\text{par}}_i^r = [0, \infty[$ when it is included, and $\overline{\mathcal{X}}_i^r / \overline{\text{par}}_i^r = \{\text{EXC}\}$ when it is excluded. In this example, $\overline{\mathcal{X}}_i^r = [0, \infty[\cup \{\text{EXC}\}$, therefore $\sup\{d(\mu, \nu) : \mu, \nu \in \overline{\mathcal{X}}_i^r \setminus \{\text{EXC}\}\} = \infty$, hence the parameter θ_i^r must be set to infinity to guaranty the triangular inequality which is a behaviour one would generally avoid. If the restricted sets are always bounded, then included-excluded distance becomes a standard distance that maps into \mathbb{R} , instead of $\overline{\mathbb{R}}$.

4.2 Illustration on the MLP example: distances

In this section, the included-excluded distances of each variable in the MLP example are modeled. For a meta-decreed or decreed variable that can be excluded, its parameter is arbitrarily set to $\theta_i^r = 3/2 \sup\{d(\mu, \nu) : \mu, \nu \in \overline{\mathcal{X}}_i^r \setminus \{\text{EXC}\}\}$.

The distance for the optimizer, which is the only meta variable, is

$$d_1^m(\overline{\sigma}, \overline{\sigma}') = \begin{cases} \sigma & \text{if } \overline{\sigma} \neq \overline{\sigma}', \\ 0 & \text{otherwise,} \end{cases} \quad (7)$$

where $\sigma > 0$ is a categorical parameter. Similarly, the distances for the neutral variables are

$$d_1^{\text{neu}}(\overline{r}, \overline{r}') = |\overline{r} - \overline{r}'|, \text{ and } d_2^{\text{neu}}(\overline{a}, \overline{a}') = \begin{cases} \gamma_1 & \text{if } (\overline{a} = \text{ReLU}, \overline{a}' = \text{Sig}) \text{ or } (\overline{a} = \text{Sig}, \overline{a}' = \text{ReLU}), \\ \gamma_2 & \text{if } (\overline{a} = \text{ReLU}, \overline{a}' = \text{Tanh}) \text{ or } (\overline{a} = \text{Tanh}, \overline{a}' = \text{ReLU}), \\ \gamma_3 & \text{if } (\overline{a} = \text{Sig}, \overline{a}' = \text{Tanh}) \text{ or } (\overline{a} = \text{Tanh}, \overline{a}' = \text{Sig}), \\ 0 & \text{if } \overline{a} = \overline{a}', \end{cases}$$

where $\gamma_1, \gamma_2, \gamma_3 > 0$ are categorical parameters. For meta-decreed variables, the included-excluded distances are

$$d_1^{\text{md}}(\overline{l}, \overline{l}') = |l - l'|$$

and

$$d_{i+1}^{\text{md}}(\bar{u}_i, \bar{u}'_i) = \begin{cases} 0 & \text{if } \bar{l} < i \text{ and } \bar{l}' < i, \\ 3/2 \left(\max(\bar{U}') - \min(\bar{U}') \right) & \text{if } (\bar{l} \geq i \text{ and } \bar{l}' < i) \text{ or } (\bar{l} < i \text{ and } \bar{l}' \geq i), \\ |\bar{u}_i - \bar{u}'_i| & \text{if } \bar{l} \geq i \text{ and } \bar{l}' \geq i, \end{cases}$$

where $i \in \{1, 2, \dots, l_{\max}\}$, $\bar{U}' = U_{\text{ASGD}} \cup U_{\text{ADAM}}$, and $\bar{l} < i$ signifies that the i -th unit is not included, whereas $\bar{l} \geq i$ signifies that it is included. Finally, the included-excluded distances for the decreed variables are given by the expressions

$$d_i^{\text{dec}}(\bar{\alpha}_i, \bar{\alpha}'_i) = \begin{cases} 0 & \text{if } \bar{o} = \text{ADAM} = \bar{o}', \\ 3/2 & \text{if } \bar{o} \neq \bar{o}', \\ |\bar{\alpha}_i - \bar{\alpha}'_i| & \text{if } \bar{o} = \text{ASGD} = \bar{o}', \end{cases} \quad \text{and} \quad d_{j+3}^{\text{dec}}(\bar{\beta}_j, \bar{\beta}'_j) = \begin{cases} 0 & \text{if } \bar{o} = \text{ASGD} = \bar{o}', \\ 3/2 & \text{if } \bar{o} \neq \bar{o}', \\ |\bar{\beta}_j - \bar{\beta}'_j| & \text{if } \bar{o} = \text{ADAM} = \bar{o}', \end{cases}$$

where $i, j \in \{1, 2, 3\}$, and

$$d_7^{\text{dec}}(\bar{\rho}, \bar{\rho}') = |\bar{\rho} - \bar{\rho}'|.$$

4.3 Graph-structured distance and induced distance

Now that the included-excluded distance has been detailed, the following theorem formally introduces the graph-structured distance.

Theorem 4 (Graph-structured distance). *For any $p \geq 1$, the graph-structured function $\overline{\text{dist}}_p : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}^+$ defined by*

$$\overline{\text{dist}}_p(\bar{x}, \bar{y}) := \left(\sum_{r \in R} \sum_{i \in I^r} d_i^r(\bar{x}_i^r, \bar{y}_i^r)^p \right)^{1/p}, \quad (8)$$

is an extended real-valued distance function, where $R = \{\text{m}, \text{md}, \text{dec}, \text{neu}\}$.

Proof. The identity of indiscernibles, nonnegativity and symmetry of $\overline{\text{dist}}_p$ are trivially proven since the operations of summation and exponentiation with $p \geq 1$ on the included-excluded distances in (8) conserve these properties. The rest of the proof consists of showing the triangular inequality is respected by demonstrating that $\overline{\text{dist}}_p$ is equivalent to a p -norm, that respects the triangular inequality. Let $K = \{1, 2, \dots, n^{\text{m}} + n^{\text{md}} + n^{\text{dec}} + n^{\text{neu}}\}$ be a set of indices that reorders the indices $r \in \{\text{m}, \text{md}, \text{dec}, \text{neu}\}$ and $i \in \{1, 2, \dots, n^r\}$:

- $a_k := d_i^{\text{m}}(\bar{x}_i^{\text{m}}, \bar{y}_i^{\text{m}})$, for $k = i$ with $i \in \{1, 2, \dots, n^{\text{m}}\}$,
- $a_k := d_j^{\text{md}}(\bar{x}_j^{\text{md}}, \bar{y}_j^{\text{md}})$, for $k = n^{\text{m}} + j$ with $j \in \{1, 2, \dots, n^{\text{md}}\}$,
- $a_k := d_l^{\text{dec}}(\bar{x}_l^{\text{dec}}, \bar{y}_l^{\text{dec}})$, for $k = n^{\text{m}} + n^{\text{md}} + l$ with $l \in \{1, 2, \dots, n^{\text{dec}}\}$,
- $a_k := d_v^{\text{neu}}(\bar{x}_v^{\text{neu}}, \bar{y}_v^{\text{neu}})$, for $k = n^{\text{m}} + n^{\text{md}} + n^{\text{dec}} + v$ with $v \in \{1, 2, \dots, n^{\text{neu}}\}$.

Finally, let $a = (a_1, a_2, \dots, a_{|K|})$, then

$$\|a\|_p = \left(\sum_{k=1}^{|K|} |a_k|^p \right)^{1/p} = \left(\sum_{r \in R} \sum_{i \in I^r} d_i^r(\bar{x}_i^r, \bar{y}_i^r)^p \right)^{1/p} = \overline{\text{dist}}_p(\bar{x}, \bar{y})$$

□

For $p \rightarrow \infty$, the graph-structured distance $\overline{\text{dist}}_\infty : \overline{\mathcal{X}} \times \overline{\mathcal{X}} \rightarrow \overline{\mathbb{R}}^+$ is defined as a maximum, *i.e.*,

$$\overline{\text{dist}}_\infty(\overline{x}, \overline{y}) := \max \{ d_i^r(\overline{x}_i^r, \overline{y}_i^r) : r \in R, i \in I^r \}, \quad (9)$$

which is trivially a distance function by virtue of the max function.

Note that, in practice, variables often require scaling to improve the conditioning and eliminate biases related to variable scales. In the context of the work, scaling categorical variables and excluded variables is ambiguous. Fortunately, in our proposed distance, an included-excluded distance d_i^r is defined with a flexible distance d for its both included case. Therefore, the distance d can be defined using a scaling parameter, such that $d(a, b) = \omega_i^r d'(a, b)$, where $\omega_i^r > 0$ is a weight parameter related to the variable \overline{x}_i^r and d' is a one-dimensional distance of appropriate variable type. The weight parameter ω_i^r can be used to automatically scale the lower bounds of the parameter θ_i^r , since the lower bound of θ_i^r is defined with the one-dimensional distance d . In Section 5, scaling parameters will be used to better adjust our proposed distance to the datasets; this helps to remove biases that are related to variable scales.

Theorem 2, which establishes the bijection between the domain \mathcal{X} and the extended domain $\overline{\mathcal{X}}$, implies that a distance $\text{dist}_p : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}^+$ can be induced from the graph-structured distance $\overline{\text{dist}}_p : \overline{\mathcal{X}} \times \overline{\mathcal{X}} \rightarrow \overline{\mathbb{R}}^+$. The following corollary is a direct consequence of Theorems 2 and 4.

Corollary 1 (Induced distance). *For $p \geq 1$, the induced function $\text{dist}_p : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}^+$ defined by*

$$\text{dist}_p(x, y) := \overline{\text{dist}}_p(T_G(x), T_G(y)) = \overline{\text{dist}}_p(\overline{x}, \overline{y}), \quad (10)$$

is an extended real-valued distance, where $\overline{\text{dist}}_p : \overline{\mathcal{X}} \times \overline{\mathcal{X}} \rightarrow \overline{\mathbb{R}}^+$ is a graph-structured distance and $T_G : \mathcal{X} \rightarrow \overline{\mathcal{X}}$ is the bijective transfer mapping.

Corollary 1 unpacks most of the contributions. To arrive at Corollary 1, it was necessary to: 1) define an extended point \overline{x} , restricted sets and the extended domain $\overline{\mathcal{X}}$ using notions from graph theory; 2) define the transfer mapping $T_G : \mathcal{X} \rightarrow \overline{\mathcal{X}}$, and prove that it is bijective, 3) define the included-excluded distances on the universal set for tackling variables that can either be included or excluded, or with different admissible values, and 4) define the graph-structured distance $\overline{\text{dist}}_p : \overline{\mathcal{X}} \times \overline{\mathcal{X}} \rightarrow \overline{\mathbb{R}}^+$ based on the contributions mentioned above.

5 Computational experiments: least-squares problems of the working example

This section compares two approaches on least-squares regression problems with simple distance-based models for instances of the MLP example. The first approach, named **Sub**, divides a regression problem into subproblems, each assigned to a portion of the domain in which the included variables are fixed. The second approach, called **Graph**, uses the induced distance in (10) with $p = 2$ to tackle a regression problem directly and by aggregating the data across the subproblems.

Table 2 from A details the five variants of the working example for the two approaches. The variants are of increasing difficulty, notably in terms of number of subproblems and

variables present. Each variant is instantiated by four distinct datasets of varying size amongst very small (VS), small (S), medium (M) and large (L). There are two levers of difficulty, the variant itself, and the amount of data available. Table 3 from B details the dataset sizes for the twenty instances, where an instance is characterized as variant-size. The computational experiments are done in a context where the amount of data is relatively limited, in order to motivate the induced distance that aggregates data.

5.1 Setup

The generation of a data couple $(x, f(x))$ is done by the following three steps: 1) a MLP model is constructed with respect to its given hyperparameters $x \in \mathcal{X}$ with PyTorch; 2) the MLP is trained and validated with 25% of the Fashion-MNIST training dataset (15k data); 3) the performance score $f(x) \in [0, 100]$, that represents the percentage of well-classified images, is computed on the MLP with another 25% of the Fashion-MNIST test dataset (2.5k data). In order to reduce data generation time, only 25% of the Fashion-MNIST dataset is used, and the number of epochs and batch size are respectively set to 25 and 128. Each instance has a heterogeneous dataset that is partitioned into a training, validation and test sets.

For **Sub**, these datasets are further divided into subproblems according to Table 3.

Two types of regression models are considered, the inverse distance weighting (IDW) and the K -nearest neighbors (KNN). For IDW, the training dataset is composed of data points and images that are used for interpolation. For KNN, the training dataset contains data points that are available as neighbors, and the images of these neighbors are used to compute a mean. **Graph** constructs a single model with an induced distance. **Sub** constructs many models, one per subproblem, and each model uses an Euclidean distance defined on their corresponding subdomain. Four approach-models are considered: **Sub-IDW**, **Graph-IDW**, **Sub-KNN** and **Graph-KNN**.

In the computational experiments, Root Mean Squared Errors (RMSE) on validation and test datasets, respectively referred to the RMSE validation and RMSE test, are computed. For **Sub**, a RMSE is computed by assigning data points to their respective subproblem and model. Before computing a RSME test, parameters are adjusted with respect to a corresponding RMSE validation. The optimization is expressed as a least-squares problem focused on minimizing the RMSE validation as the objective function, where the decision variables are the parameters of a specified approach-model. The parameters to adjust depend on the model type and the approach employed. Regarding the model, IDW adds no parameter, whereas KNN adds the number of neighbors K for **Graph** and a number of neighbors per subproblem for **Sub**. Both approaches have weight parameters as discussed in Section 4.3. **Graph** also requires parameters for the excluded-included distances between variables that can take the special value **EXC**, and a parameter for the categorical distance of the optimizer (in the situations where the categorical distance is not fixed). The optimization of the RMSE validation is done with the open-source blackbox optimization software **NOMAD** [9] that is based on the Mesh Adaptive Direct Search algorithm [6] (MADS). RMSE tests are used to assess the generalization ability of the approach-models, and they are not subject to any optimization.

5.2 RMSE validation and test

Table 1 presents the final RMSE validation and test obtained for the approach-models on each instance, characterized by a variant and dataset size. In Table 1a, the RMSE validation value is the smallest value obtained during its optimization. In Table 1b, the RMSE test value is evaluated with the best parameters obtained, *i.e.*, the ones corresponding to the smallest RMSE validation value. For each table and instance (row), the smallest value obtained by a approach-model appears in bold.

Var.	Size	IDW		KNN	
		Sub	Graph	Sub	Graph
#1	VS	12.45	12.64	17.50	5.08
	S	14.58	11.62	21.29	4.65
	M	11.49	11.51	7.75	7.93
	L	9.18	9.18	16.43	5.87
#2	VS	17.21	17.03	20.80	11.95
	S	16.78	17.63	22.42	9.11
	M	17.67	16.53	16.90	9.63
	L	16.95	16.72	18.19	8.46
#3	VS	16.59	14.57	15.53	10.96
	S	13.65	13.98	18.25	10.26
	M	12.52	13.22	10.93	13.19
	L	12.71	12.50	12.81	12.36
#4	VS	13.43	14.16	21.05	13.90
	S	11.76	12.05	17.35	11.29
	M	12.11	12.46	13.00	10.14
	L	12.79	13.23	16.97	10.80
#5	VS	15.86	14.13	20.87	7.52
	S	12.03	12.61	19.49	9.73
	M	13.73	14.32	15.60	12.31
	L	14.67	14.52	15.68	11.85

(a) RMSE validation (objective function).

Var.	Size	IDW		KNN	
		Sub	Graph	Sub	Graph
#1	VS	16.17	17.06	24.00	23.79
	S	13.67	13.95	27.39	19.66
	M	13.12	13.14	9.78	16.92
	L	9.32	9.32	19.77	6.39
#2	VS	14.63	14.35	21.16	15.24
	S	18.81	18.67	28.42	10.29
	M	21.54	22.03	25.71	15.54
	L	15.59	15.17	19.92	11.68
#3	VS	22.92	15.09	17.92	13.64
	S	13.62	13.53	19.30	14.05
	M	19.56	18.70	20.35	18.10
	L	13.93	13.72	15.28	16.65
#4	VS	17.68	18.10	29.54	17.56
	S	14.64	16.33	21.17	13.08
	M	18.35	18.19	23.60	17.13
	L	12.92	13.32	18.51	10.70
#5	VS	17.43	16.03	23.40	15.17
	S	13.63	13.97	21.56	13.21
	M	17.05	17.88	17.66	16.67
	L	14.99	14.55	18.46	13.74

(b) RMSE test.

Table 1: Final RMSE validation and test for budgets of 1500, 2000, 2500, 3000 and 3500 NOMAD evaluations respectively for variants 1, 2, 3, 4 and 5.

For the RMSE validation, **Graph-KNN** outperforms on most instances. In terms of approaches, **Sub-IDW** and **Graph-IDW** produce comparable results, whereas **Graph-KNN** greatly outmatches **Sub-KNN**. For the RMSE test, the conclusions are similar, but **Graph-KNN** is not as dominant. Globally, the **Graph-KNN** provides better generalization, which is not surprising, since it uses the data across all subproblems, and should therefore theoretically yield better generalization.

Graph requires more time to generate the results in Table 1, since the interpolation (IDW) or the selection of neighbors (KNN) is done on all points. The worst time gap between the two approaches has been obtained on the #5 variant with large dataset for the IDW model: approximately 10 vs 40 minutes of CPU time to run the 3,500 budget of evaluations with a 11th generation Intel i7-11800H (2.30 GHz) CPU.

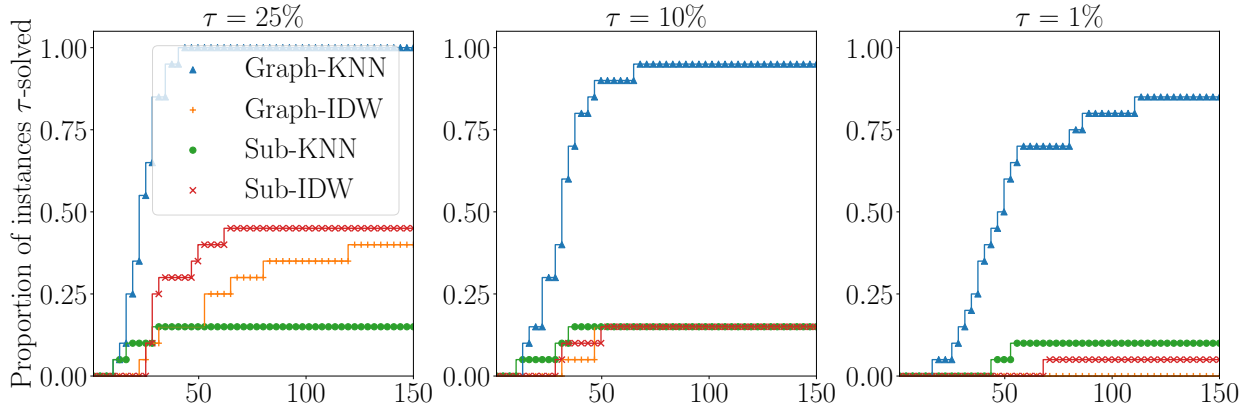
5.3 Data profiles

In this section, data profiles, which represent the proportion of τ -solved instances, are done on the approach-models for the twenty instances of the working example. An instance is said to be τ -solved by an approach-model when the convergence criteria is met within the budget of evaluations, i.e., when the relative error is within the tolerance $\tau \in \{25\%, 10\%, 1\%\}$ with respect to the best RMSE obtained by any approach-model on this instance. The fewer evaluation an approach-model requires to meet the convergence criteria, the better it has performed on that instance. The data profiles are done by following the guidelines of the derivative-free optimization community [29]. The vertical axis is the proportion of τ -solved instances and the horizontal axis is the group of evaluations, which represents the budget of evaluations allowed. The group of evaluations $(n_{p,s} + 1)$ considers the instance $p \in \{1, 2, \dots, 20\}$ and the approach-model $s \in \{\text{Sub-IDW}, \text{Graph-IDW}, \text{Sub-KNN}, \text{Graph-KNN}\}$ since the number of parameters (decision variables) depends on both the instance and approach-model. See Appendix A.3. (Data Analysis) in [8] for more details on data profiles. The data profiles are done for both the RMSE validation (objective function) and the RMSE test. Note that the optimization problem is strictly done on the RMSE validation. RMSE tests are evaluated each time that an improvement on the RMSE validation is found, in order to build the data profiles for the RMSE tests.

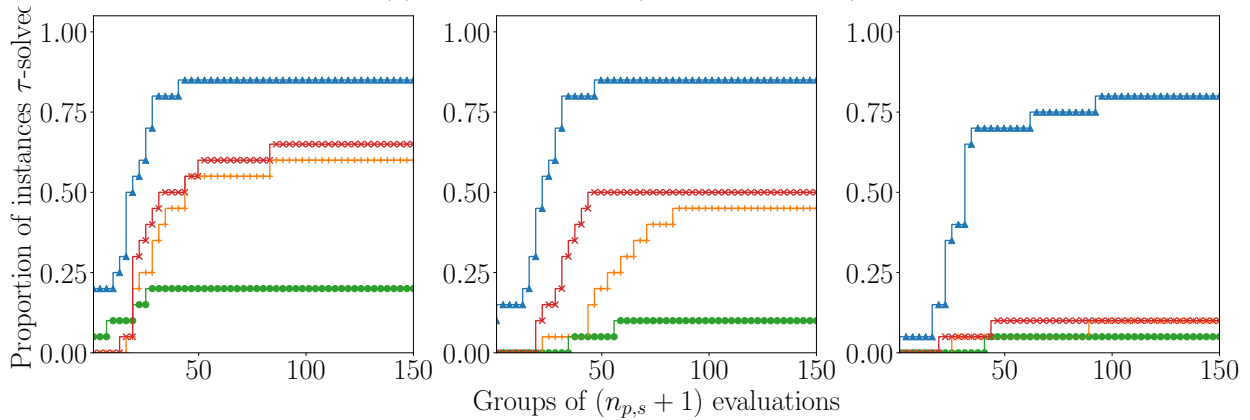
The data profiles for the RMSE validation and test clearly indicates that the **Graph-KNN** outperforms the other approach-models. For example, the data profile in Figure 4b with $\tau = 1\%$ shows that **Graph-KNN** τ -solves 5% of the instances with $10(n_{p,s} + 1)$ evaluations, and after $100(n_{p,s} + 1)$ evaluations it τ -solves 80% of the instances, whereas **Sub-KNN** only τ -solves 5%. The **Sub-IDW** and **Graph-IDW** have similar profiles, but **Sub-IDW** seems to perform slightly better. Finally, the **Sub-KNN** provides the worst performance, especially in comparison to its counterpart **Graph-KNN**.

6 Discussion

The present work focused on heterogeneous datasets that are intrinsically related to mixed-variable domains with meta and meta-decreed variables. The first important contribution, introduced in Section 3, is a generalized modeling framework for such domains, called graph-structured. The modeling framework is rigorously constructed through graph theory, and it introduces many definitions and structures, such as meta-decreed variables, the role graph $G = (V, A)$, excluded variables, extended points and the extended domain. As such, the paper generalizes the following state-of-the-art frameworks: mixed-variable domains with (strictly) meta variables [7]; tree-structured spaces [14]; hierarchical spaces [22]; variable-size design space [10, 32]; and conditional search space (or neural architecture search) [24]. The second important contribution, detailed in Section 4, concerns distance functions, which allows computation of distances between mixed-variable points that do not share the same variables. The graph-structured distance considers both the included and excluded variables in an extended point, and is constructed variable-wise with one-dimensional included-excluded to facilitate computations. Computational experiments on least-squares problems of the working example are done in Section 5. The graph-structured approach (**Graph**) ag-



(a) RMSE validation (objective function).



(b) RMSE test.

Figure 4: Data profiles for the RMSE validation and test.

gregates data across subproblems, and outperforms the approach that separates a problem into subproblems for the KNN model. Theoretically, the graph-structured approach should yield better generalizability, since it allows to use more data simultaneously: the results on the RMSE test seem to confirm this. However, further computational experiments on diverse problems and models are required to confirm that the modeling framework and the graph-structured distance are state-of-the-art for mixed-variable domains with meta variables. For instance, Gaussian processes are commonly used for such problems [32, 39, 40], and they will be studied in future works. In the near future, time consumption will also be studied more thoroughly with more complex models, and Bayesian optimization will be carried out on optimization problems with mixed-variable domains with meta variables.

Data availability statement

Scripts and data are publicly available at https://github.com/bbopt/graph_distance.

Declaration of interest statement.

On behalf of all authors, the corresponding author states that there is no conflict of interest.

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Appendix

A Variants of the working example.

In this appendix, Table 2 details the variants of the working example.

Variant #1 fixes the optimizer, hence the number of hidden layers is meta instead of meta-decreed. There are 3 subproblems, each assigned to a fixed number of hidden layers. Variant #2 adds the hyperparameters $\alpha_{1:3}$ to the first instance. Variant #3 frees the optimizer $o \in \{\text{ASGD}, \text{ADAM}\}$, and the hyperparameters $\beta_{1:3}$ are introduced via $o = \text{ADAM}$. There are 4 subproblems, each assigned to a pair (o, l) . Variant #4 adds a subproblem by allowing $l = 3$ when $o = \text{ADAM}$. The number of hidden layers l becomes a meta-decreed variable, since $L_{\text{ASGD}} \neq L_{\text{ADAM}}$. Variant #5 adds the dropout ρ with bounds in (1).

B Dataset sizes of the instances.

In this appendix, Table 3 details the dataset sizes of all instances for the two approaches.

In Table 3b, the values in size-related columns are the sums of the values in the rows of the corresponding columns in Table 3a, *i.e.*, Graph aggregates the data of the subproblems of Sub.

Var.	o	l	Variables	# of variables
#1	ASGD	1	$r \ u_1$	2
		2	$r \ u_{1:2}$	3
		3	$r \ u_{1:3}$	4
#2	ASGD	1	$r \ u_1 \ \alpha_{1:3}$	5
		2	$r \ u_{1:2} \ \alpha_{1:3}$	6
		3	$r \ u_{1:3} \ \alpha_{1:3}$	7
#3	ASGD	1	$r \ u_1 \ \alpha_{1:3}$	5
		2	$r \ u_{1:2} \ \alpha_{1:3}$	6
#3	ADAM	1	$r \ u_1 \ \beta_{1:3}$	5
		2	$r \ u_{1:2} \ \beta_{1:3}$	6
#4	ASGD	1	$r \ u_1 \ \alpha_{1:3}$	5
		2	$r \ u_{1:2} \ \alpha_{1:3}$	6
	ADAM	1	$r \ u_1 \ \beta_{1:3}$	5
2		$r \ u_{1:2} \ \beta_{1:3}$	6	
3		$r \ u_{1:3} \ \beta_{1:3}$	7	
#5	ASGD	1	$r \ u_1 \ \alpha_{1:3} \ \rho$	6
		2	$r \ u_{1:2} \ \alpha_{1:3} \ \rho$	7
	ADAM	1	$r \ u_1 \ \beta_{1:3} \ \rho$	6
2		$r \ u_{1:2} \ \beta_{1:3} \ \rho$	7	
3		$r \ u_{1:3} \ \beta_{1:3} \ \rho$	8	

(a) Variants for the Sub approach.

Var.	Variables	# of variables	# of θ_i^r
#1	$l, r, u_{1:3}$	5	2
#2	$l, r, u_{1:3}, \alpha_{1:3}$	8	2
#3	$o, l, r, u_{1:2}, \alpha_{1:3}, \beta_{1:3}$	11	7
#4	$o, l, r, u_{1:3}, \alpha_{1:3}, \beta_{1:3}$	12	8
#5	$o, l, r, u_{1:3}, \alpha_{1:3}, \beta_{1:3}, \rho$	13	8

(b) Variants (Var.) for the Graph approach.

Table 2: Variants of the working example with $u_{1:2} = (u_1, u_2)$, $u_{1:3} = (u_1, u_2, u_3)$, $\alpha_{1:3} = (\alpha_1, \alpha_2, \alpha_3)$ and $\beta_{1:3} = (\beta_1, \beta_2, \beta_3)$; the activation function is fixed at $a = \text{ReLU}$ for all variants.

Variant	o	l	VS	S	M	L
#1	ASGD	1	20	30	40	50
		2	30	45	60	75
		3	40	60	80	100
#2	ASGD	1	50	75	100	125
		2	60	90	120	150
		3	70	105	140	175
#3	ASGD	1	50	75	100	125
		2	60	90	120	150
	ADAM	1	50	75	100	125
		2	60	90	120	150
#4	ASGD	1	50	75	100	125
		2	60	90	120	150
	ADAM	1	50	75	100	125
		2	60	90	120	150
		3	70	105	140	175
		3	70	105	140	175
#5	ASGD	1	60	90	120	150
		2	70	105	140	175
	ADAM	1	60	90	120	150
		2	70	105	140	175
		3	80	120	160	200
		3	80	120	160	200

(a) Dataset sizes for Sub approach.

Variant	VS	S	M	L
#1	90	135	180	225
#2	180	270	360	450
#3	220	330	440	550
#4	290	435	580	725
#5	340	510	680	850

(b) Dataset sizes for Graph approach.

Table 3: Dataset sizes of the instances, characterized by a variant-size, with sizes amongst very small (VS), small (S), medium (M) and large (L).

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