Conjecturing-Based Discovery of Patterns in Data*

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We propose the use of a conjecturing machine that generates feature relationships in the form of bounds involving nonlinear terms for numerical features and boolean expressions for categorical features. The proposed Conjecturing framework recovers known nonlinear and boolean relationships among features from data. In both settings, true underlying relationships are revealed. We then compare the method to a previously-proposed framework for symbolic regression and demonstrate that it can also be used to recover equations that are satisfied among features in a dataset. The framework is then applied to patient-level data regarding COVID-19 outcomes to suggest possible risk factors that are confirmed in medical literature.

Key words: automated conjecturing, computational scientific discovery, interpretable artificial intelligence, nonlinear pattern discovery, boolean pattern discovery

History:

1. Introduction

Modern machine learning methods allow one to leverage complex relationships present in data to generate accurate predictions but do not reveal them to the investigator (Section 3). We propose an automated conjecturing framework for discovering nonlinear and boolean relationships among the features in a given dataset. Our primary goal is discovery - to provide the investigator with a manageable number of suggested relationships to inspire future investigation for validation.

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The nonlinear relationships are produced in the form of bounds. Bounds are useful for scientific discovery from numeric data because they 1) suggest direct and indirect relationships among features, 2) suggest a functional form for the relationships, and 3) can subsequently be used as boolean features (e.g., is this bound satisfied by an observation?) for discovering more complex boolean relationships. Whereas previous related approaches seek to find equations for numeric data, our Conjecturing method produces bounds for numeric data, boolean expressions for discrete data, and bounds and boolean expressions for mixed data.

Udrescu and Tegmark (2020) proposed a system called AI FEYNMAN that combines deep learning with methods for symbolic regression to recover nonlinear relationships in data. Impressively, they recover over 100 equations of varying complexity from data. In contrast to AI FEYNMAN, our Conjecturing framework uses Fajtlowicz's Dalmatian heuristic (Fajtlowicz 1995) to discover bounds rather than equations. Further, our framework can also be applied to categorical data to discover boolean relationships among features and already-discovered bounds. This work represents the first application of the Dalmatian heuristic to learning both nonlinear and boolean relationships from data. The bounds and conditions produce interpretable yet complex relationships.

2. Background and Previous Related Work

In this section, we provide background on our Conjecturing framework including examples of uses of bounds and sufficient conditions, a description of the core algorithm, and a survey of previous related work.

2.1. Motivating Examples for Conjectured Bounds and Sufficient Conditions

The algorithm we use to conjecture feature relationships is an adaptation of an algorithm that was originally designed to conjecture relationships for mathematical objects. To illustrate the potential value of bounds and sufficient conditions, we describe two problems and relevant results from graph theory. This paper extends these ideas regarding bounds and sufficient conditions to learning from data.

A graph is a collection of nodes V and edges E that are ordered pairs of nodes. Consider the problem of finding bounds for the independence number of a graph¹. It is well known that the linear programming (LP) relaxation of an appropriate integer program provides a upper bound on the independence number (Schrijver 2003). The Lovász ϑ number of a graph also provides an upper bound that is known to be no larger than the LP relaxation bound for any graph (Lovász 1979). Therefore, the Lovász ϑ bound dominates the LP relaxation bound, and such relationships are

¹ The independence number is the largest number of nodes in a graph no two of which are contained in an edge. The definition of independence number is not important for this example, but only the fact that with every graph is associated a number called the "independence number".

commonly pursued. However, relationships among bounds can be more nuanced. Consider a third bound on the independence number due to Haemers (1979). For some graphs it is a stronger bound than Lovász ϑ while on other graphs it is a weaker bound; for some graphs, Lovász ϑ is a sharp bound and Haemers's bound is not while for other graphs, Haemers's bound is a sharp bound and Lovász ϑ is not. It remains an open question whether there are a "small" number of bounds where the largest for value for any graph would provide a sharp bound on the independence number. In this paper, we describe a computational approach to discover bounds among numeric features in a dataset. As with the independence number, collections of bounds can provide valuable insight into relationships for the system from which the data was collected.

Now consider the problem of finding sufficient conditions for a graph to be Hamiltonian². Chvátal (1972) proved that for a graph G with certain conditions on the vertex degrees, G is Hamiltonian. Also, Chvátal and Erdös (1972) proved that if a graph satisfies a connectivity condition, then it is Hamiltonian. These are two conditions that are sufficient for a graph to be Hamiltonian, but neither implies the other. Some graphs satisfy both conditions, some graphs satisfy one condition, and some graphs satisfy neither condition. The existence and discovery of a (small) set of sufficient conditions that characterize all Hamiltonian graphs remains an open area of research. The pursuit of sufficient conditions of graph properties such as Hamiltonicity mirrors that of bounds (Larson and Van Cleemput 2017). In the context of learning from data, we show how categorical data, together with bounds discovered among numeric features, can be used as input to a computational approach for generating sufficient conditions for a property of interest.

2.2. The Dalmatian Heuristic

Our Conjecturing framework is based on an implementation of Fajtlowicz's Dalmatian heuristic (Fajtlowicz 1995, Larson and Van Cleemput 2017). The heuristic was originally implemented in Graffiti (Fajtlowicz 1995) which was the first program to produce research conjectures that led to new mathematical theory. The program produces statements that are relations between mathematical *invariants* which are numerical attributes of examples. Recent implementations of the Dalmatian heuristic have been applied to the discovery of relationships for graphs (Larson and Van Cleemput 2016) and game strategies (Bradford et al. 2020). The heuristic was adapted to work with *properties* which are boolean attributes of examples by Larson and Van Cleemput (2017). We built our framework using a more recent implementation of the Dalmatian heuristic available here: http://nvcleemp.github.io/conjecturing/.

We now describe invariant conjecturing using Fajtolwicz's Dalmatian heuristic. The inputs include the following. Let E be a set of examples of a given type (e.g., graphs or data observations).

² A Hamiltonian graph is a graph with a spanning cycle (West 2001). The definition of Hamiltonian is not important for this example, but only the fact that any graph either is or is not Hamiltonian.

Let $A = \{\alpha_1, \alpha_2, \dots, \alpha_m\}$ be real number invariants. In this work the examples are n data observations and the invariants are m numeric features. The real-numbered value of example i for invariant α_j is $\alpha_j(i) = x_{ij}$ for $i = 1, \dots, n$ and $j = 1, \dots, m$. Let O be a collection of unary operators and binary operators. Examples of unary operators include adding 1, squaring, square-rooting, and division by 2. Binary operators include addition, multiplication, and subtraction. Let $\alpha^* \in A$ be the invariant for which upper and lower bounds are of interest, and let $\alpha^*(i)$ be the value of the invariant of interest for example i.

The aim is to generate conjectured bounds that are true for any realization of input examples E. The Dalmatian heuristic provides criteria for generating conjectured bounds that are the best for E. Algorithm 1 provides a way to generate expressions of increasing complexity, apply the heuristic, and store conjectures. The *complexity* of an expression is the number of nodes in the corresponding expression tree (Figure 1) and is the sum of the number of invariants, number of unary operators, and number of binary operators. The algorithm proceeds by generating unlabeled trees and then labeling the nodes with operators and invariants. Expressions satisfying the Dalmatian heuristic conditions are retained as conjectures C. For a conjecture c, let c(i) be the conjectured bound for example i.

With examples E, invariants A, operators O, invariant of interest α^* , an upper limit on the proportion of missing values allowed for an invariant skips, and a direction indicating if the algorithm will produce upper or lower bounds (UPPER or LOWER), **procedure** Conjecturing-INV is called (Algorithm 1, line 1). The number of unary nodes u and binary nodes b of an expression tree are initialized to zero and the conjectures C is initialized to the empty set (Algorithm 1, line 2). Line 3 of Algorithm 1 refers to the stopping criteria of the expression generator. For invariant conjecturing for upper bounds, if the minimum conjectured bound is tight for each example (i.e., $\min_{c \in C} c(i) = \alpha^*(i)$ for $i \in E$), then the expression generator is stopped. Otherwise, expression generation continues until a time limit is reached. Line 4 calls a procedure to generate a tree, the branching nodes of which will be operators and the leaf nodes are invariants. Lines 5-11 help to enumerate every tree where each vertex connected to a leaf node has degree one or two. These branching nodes will correspond to unary or binary operators, respectively, when the tree is labeled. The leaf nodes will correspond to invariants. Unlabeled trees are grown recursively and then the nodes are labeled with operators and invariants.

The **procedure** GENERATETREE (Algorithm 1, line 4) creates a new tree with a single node, then calls **procedure** GENERATETREEREC to add new nodes until there are u unary nodes and b binary nodes. The **procedure** GENERATETREEREC (Algorithm 1, line 19) either calls GENERATE-LABELEDTREE to apply labels by assigning invariants to leaf nodes and operators to branching nodes to generate an expression (Algorithm 1, line 21), or adds nodes to grow the tree (lines 23-32).

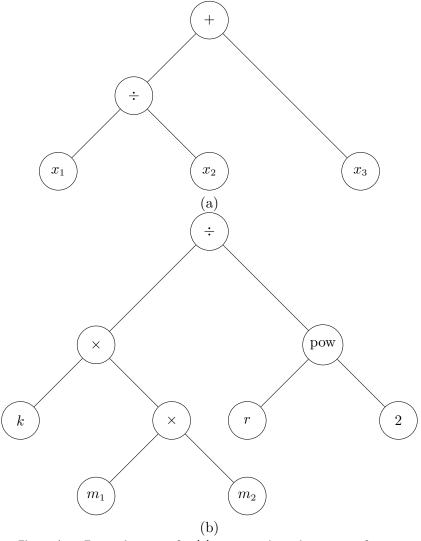


Figure 1 Expression trees for (a) an upper bound on square footage $x_1/x_2 + x_3$ where x_1 is 300K, x_2 is pricePerSquareFoot, and x_3 is bathrooms and (b) gravitational force km_1m_2/r^2 .

The **procedure** GENERATELABELEDTREE (Algorithm 1, line 35) takes as input a tree with u unary nodes and b binary nodes. Line 36 orders the children nodes in the order left to right appear before their parent. Then line 37 creates a set of labeled trees. The leaf nodes are labeled with invariants and the branching nodes are labeled with operators. Invariants with more than skips missing values among examples are not used for labeling. For the commutative binary operators, the left child is larger than the right if the left has more nodes. If the number of nodes is equal, we use the lexicographically largest string of labels. Since the suffix order guarantees that all subtrees are fully labeled before their parent is labeled, this is an unambiguous definition. Examples of labeled expression trees are given in Figure 1.

Lines 39 and 41 are the Dalmatian heuristic. A conjectured upper bound c is only retained in the database of conjectures C if the bound passes the following two tests:

- 1. (Truth test). The candidate conjecture $\alpha^*(i) \leq c(i)$ is true for all examples $i \in E$, and
- 2. (Non-dominance test.) There is an example i where $c(i) < \min\{c'(i) : c' \in \mathcal{C} \setminus \{c\}\}$. That is, the candidate conjecture would give a better bound for $\alpha^*(i)$ than any previously conjectured (upper) bound.

Line 41 ensures that the number of conjectures is no larger than the number of examples; i.e., $|\mathcal{C}| \leq |E|$.

The procedure is the same for generating lower bounds with the only difference being how the Dalmatian heuristic criteria are evaluated in lines 39 and 41.

The computational requirements of Algorithm 1 increase exponentially with the number of invariants and with the number of operators. The computation time increases with the number of examples because of the check in Step 39. To facilitate generation of more candidate expressions in less time, one can use fewer examples as input to the algorithm. To achieve additional efficiency, we implement the following design choice. In our implementation, when a tree is labeled, operators can be reused, but invariants cannot. We make this design choice so that more expressions can be generated in a smaller amount of time. In Section 5.4, we will demonstrate how this limitation can be overcome in situations where repeating invariants is warranted.

Figure 2 displays (a) upper bounds and (b) lower bounds derived for test instances for data generated based on a formula for gravity. The gray curves correspond to bounds, and each must be the best on at least one training example instance in order to be retained. More details on this experiment are provided in Section 3.1 and Section 4.1.

Algorithm 1 can be adapted for property conjecturing with few modifications. We now detail the differences. Let E be a set of examples and let $\Pi = \{\pi_1, \pi_2, \dots, \pi_m\}$ be properties. The examples are n data observations and the properties are m boolean features. The truth value of example i for property π_j is $\pi_j(i)$. Let O be the following collection of operators: NOT (\neg) , AND (&), OR (|), XOR (exclusive or) (\oplus) , and IMPLIES (\rightarrow) . NOT is a unary operator and the remaining operators are binary operators. Let $\pi^* \in \Pi$ be the property for which sufficient and/or necessary conditions are of interest, and let $\pi^*(i)$ be the truth value of the property of interest for example i.

The aim is to generate conjectured sufficient or necessary conditions for the property of interest that are valid for any realization of input examples E. The algorithm for property conjecturing **procedure** Conjecturing-PROP generates unlabeled trees as in Algorithm 1 but then labels the nodes with operators and properties. Logical expressions satisfying the Dalmatian heuristic conditions are retained as conjectures C. For a conjecture c, let c(i) be the conjectured truth value for example i.

The inputs to property conjecturing are examples E, properties Π , operators O, a property of interest π^* , and a direction (SUFFICIENT, NECESSARY) indicating if the algorithm will produce sufficient or necessary conditions for the property of interest.

Algorithm 1 Invariant Conjecturing.

Input: Examples E, Invariants A, operators O, invariant of interest α^* , invariant missing value limit skips, direction (UPPER or LOWER).

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Output: Conjectured C in the form of conjectured bounds on the invariant of interest \alpha^*.
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```
1: procedure Conjecturing-INV
       Set u = 0, b = 0, C = \emptyset.
3:
       \mathbf{while} not stopped \mathbf{do}
4:
          GENERATETREE(u, b).
5:
          if b = 0 then
6:
              Set b = \lceil u/2 \rceil.
7:
              Set u = 0.
8:
          else
9:
10:
              u + = 2.
11:
           end if
12:
       end while
13:
       return C.
14: end procedure
15: procedure GENERATETREE(u, b)
16:
       Set tree = new tree with single node.
17:
       GENERATETREEREC(tree, u, b).
18: end procedure
19: procedure GENERATETREEREC(tree, u, b)
20:
       if number of unary nodes == u and number of binary nodes == b then
21:
           GENERATELABELEDTREE(tree).
22:
23:
          for all nodes v on the second-deepest level that have at most 1 child and have no nodes at the same level to their
   right with at least 1 child \mathbf{do}
24:
              Add child to v.
25:
              GENERATETREEREC(tree, u, b).
26:
              Remove that child from v.
27:
           end for
28:
           for all nodes v on the deepest level do
29:
              Add child to v.
30:
              GENERATETREEREC(tree, u, b).
31:
              Remove that child from v.
32:
           end for
33:
       end if
34: end procedure
35: procedure GENERATELABELEDTREE(tree)
36:
       Order the nodes in a suffix order.
37:
       Recursively label each node in this ordered array with either an invariant, a unary operator, or a binary operator
   depending on its degree. For commutative binary operators we only label a vertex if its left child is larger than its right
38:
       for each fully labeled tree do
39:
          if the corresponding bound c is valid for all examples in E and is not dominated by existing bounds in C. then
40:
              Set C = C \cup c.
41:
              Remove dominated conjectures from C.
42:
           end if
43:
       end for
44: end procedure
```

The stopping criterion for property conjecturing for the case that direction is SUFFICIENT is obtaining a set of conjectures where for every example with $\pi^*(i) = \text{true}$, each example evaluates to true for at least one conjecture. Otherwise, expression generation continues until a time limit is reached.

The Dalmatian heuristic for property conjectures is applied as follows. A conjectured sufficient condition c is only retained in the database of conjectures C if the expression passes the following two tests:

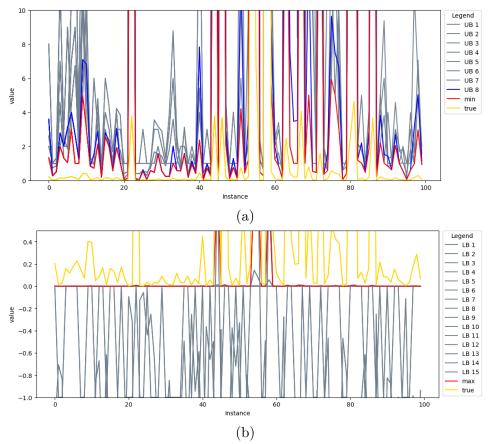


Figure 2 (a) Upper bounds and (b) lower bounds generated for gravitational force using Conjecturing-INV, the invariant version of the conjecturing algorithm. Instances from the training data are on the *x*-axis. The gold curve is the true value for the instances. The blue curve in (a) is the true value without the constant of proportionality and is one of the upper bounds. The red curve is the (a) maximum and (b) minimum of the discovered bounds.

- 1. (Truth test). For all examples $i \in E$ for which c(i) is true, then $\pi^*(i)$ is also true, and
- 2. (Non-dominance test.) The number of examples $i \in E$ for which c(i) is true is not a subset of examples that evaluate to true for any previously conjectured sufficient condition.

To generate necessary conditions for π^* , one can generate sufficient conditions for $\neg \pi^*$ (NOT π^*).

Figure 3(a) depicts candidate conditions for examples with the property of interest (green) and those without (red). Conditions 1 and 2 are sufficient conditions for subsets of examples with the property of interest. Condition 3 evaluates to true for examples with and without the property of interest, and would therefore not be retained. The goal of property conjecturing is to find a set of sufficient conditions that evaluate to true for all examples with the property of interest and for none of the examples without the property of interest as illustrated in Figure 3(b).

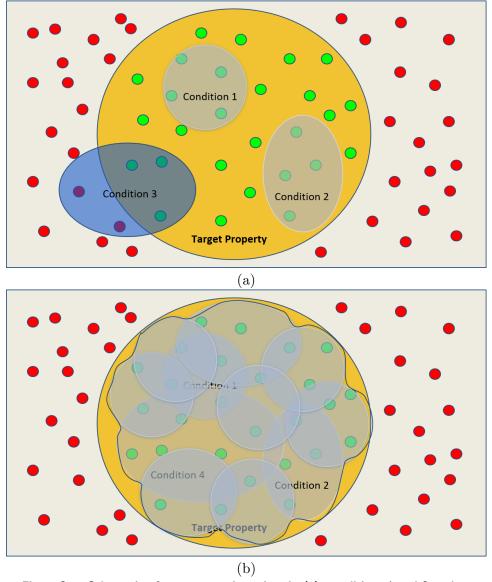


Figure 3 Schematic of property conjecturing. In (a), conditions 1 and 2 evaluate to true for a subset of examples with the property of interest and for no samples that do not have the property of interest. Condition 3 evaluates to true for examples with and without the property of interest, and so it is discarded. In (b), the union of sufficient conditions covers all examples with the property of interest.

2.3. Other Related Work

In this section, we explain how our work is related to previous work in automated scientific discovery, machine learning interpretability, automated feature engineering, and empirical model building.

Symbolic regression has been used as a tool for automated scientific discovery. Symbolic regression is the use of genetic programming to approximate a target function on training data and generalize to produce predictions on new data (Nicolau and Agapitos 2021) and until the work of Schmidt and Lipson (2009), the focus was on improving prediction accuracy by approximating an underlying function rather than a focus on discovering true functional relationships among fea-

tures. Schmidt and Lipson (2009) extend previous work to develop a system for discovering laws for dynamical systems by considering relationships among derivatives. Their work led to the development of a software Eureqa. More recently, Udrescu and Tegmark (2020) combined a variety of strategies including dimensional analysis, symmetry identification, neural network training, and brute-force enumeration into a framework called AI Feynman to recover true physical functional forms from data. Petersen et al. (2021) propose a method for deep symbolic regression that combines reinforcement learning with a recurrent neural network model. They compare their approach with methods based on priority queue training proposed by (Abolafia et al. 2018) and the traditional genetic programming approach. Our experiments include comparisons with each of these methods in the ability to recover equations from data.

Other frameworks have been proposed to computationally generate conjectures from data and discover scientific laws. Data smashing is introduced by Chattopadhyay and Lipson (2014) as a method for computing dissimilarities from streams of data (e.g., electroencephalogram data) to aid in revealing relationships among observations. Jantzen (2020) proposes an algorithm with the similar purpose of detecting types of dynamical systems called *dynamical kinds*. Subsequently, these kinds "are then targets for law-like generalization" (Jantzen 2020). While Jantzen's work provides a method for discovering the kinds, it does not suggest how to recover the "laws". It is these relationships that we aim to discover with the Conjecturing framework.

Our work is distinguished from these previous works in that 1) we focus on generating bounds for invariants that serve as hypotheses for the investigator rather than recover true functional forms or generate accurate predictions, 2) our invariant conjecturing algorithm is paired with a property conjecturing algorithm for discovering both nonlinear bounds and boolean relationships, 3) our framework is designed for a given static observational dataset rather than on discovering laws for dynamical systems, and 4) rather than a stochastic search over the space of functional forms, our Conjecturing system leverages sophisticated techniques for enumerating expressions of increasing complexity (described in Larson and Van Cleemput (2016) for "noiseless" data involving mathematical objects such as graphs). In our system, the human remains "in the loop" to evaluate the plausibility of suggested bounds and conditions.

Brunton et al. (2016) introduce SINDY for combining sparse regression and expert knowledge to developing models of dynamical systems. We adopt a similar approach to incorporating prior knowledge in Section 5.4 for the Nguyen benchmark suite (Nguyen et al. 2011) where we provide the Conjecturing framework with candidate non-linear functions as building blocks. Unlike our Conjecturing framework, theirs is designed for recovering equations governing dynamical systems rather than bounds and theirs is not capable of recovering boolean relationships.

Langley (2019) provides a review of past efforts in computational scientific discovery. Several frameworks have their origins in analyzing mass spectroscopy and other electrochemical data. Bacon (Langely et al. 1987) is a general framework for scientific discovery based on suggesting and executing a series of designed experiments. Tallorin et al. (2018) proposed a method called POOL that uses Bayesian optimization and machine learning in an iterative fashion for experiments to discover peptide substrates for enzymes. Bacon and POOL both make recommendations regarding additional data to collect while our system assumes that a fixed dataset is provided that may or may not be the result of a designed experiment.

Precise definitions of "explainability" and "interpretability" are still being developed (Vilone and Longo 2020, Lu et al. 2019, Fürnkranz et al. 2020) as research in the area has rapidly accelerated. According to the convention of Rudin (2019), explainability is concerned with post-hoc analyses of black box models to create simple explanations of model behavior. Motivated by observed accuracies of deep learning models, work in this area includes identifying important features for prediction, building simple local models, conducting sensitivity analyses, and deriving prototype examples (Samek and Müller 2019, Elton 2020). Tsang et al. (2018a,b, 2020) develop neural network frameworks for identifying sets of features for which there is an *interaction* - a non-additive relationship among predictive features that influence a response value. These methods provide explainability in that they identify sets of features that interact, but the framework is not designed to reveal the functional form of the nonlinear interaction.

Rudin (2019) advocates the development of interpretable models where the mechanisms for predictions are simple relationships that are readily apparent to the investigator. Much of the recent work in this area is in the development of decision rules (e.g., (Hammer and Bonates 2006, Dash et al. 2018, Bellomarini et al. 2020)) or decision lists and trees (e.g., (Wang and Rudin 2015, Wang et al. 2017, Rudin and Ertekin 2018, Bertsimas and Dunn 2017, Verwer and Zhang 2019, Blanquero et al. 2021, Aghaei et al. 2021, Akyüz and Birbil 2021)). Different from these works, our Conjecturing framework automates the discovery of nonlinear features. In addition, as with work on decision rules in general, our framework can combine the discrete features in data with the discovered nonlinear features to discover a potentially richer set of boolean relationships when compared to optimization-based trees and decision lists.

Khurana et al. (2018) propose a system that leverages reinforcement learning to search expression trees for predictive features. ExploreKit (Katz et al. 2016) is a framework for automatic feature engineering that combines features using basic arithmetic operations and then uses machine learning to rank and select those with high predictive ability. The Data Science Machine (Kanter and Veeramachaneni 2015) automatically generates features for entities in relational databases with possible dependencies between tables followed by singular value decomposition. In none of

these works is model transparency evaluated but rather only model performance. An important distinction of our work from these is that they focused on improving prediction accuracy, sometimes at the expense of understandable features, and not on scientific discovery.

Traditional statistical methods for empirical model building (e.g. regression analysis) tend to focus on first- and second-order polynomial models; interaction terms up to a certain degree are often included. Empirical models are intended to provide adequate prediction performance while also providing a simple assessment of feature importance via model coefficients. Techniques such as all-subsets, stepwise selection, and regularization methods (e.g., LASSO (Tibshirani 1996)) are commonly used to perform feature selection over model spaces of increasing complexity. However, domain knowledge is typically required for reciprocal or non-polynomial relationships. Our Conjecturing framework provides a search over a much broader class of nonlinear functions.

3. Two Motivating Examples

In this section, we describe two datasets where a "typical" knowledge discovery workflow fails to reveal important relationships among features.

Research on machine learning does, of course, lead to conjectured relationships between variables which are in turn used to make predictions of one or more variables in terms of others. A trained neural net, for instance, can be viewed as a black box representing a function which produces an output for every input in its domain. These functions are complex and of a different character than classical scientific laws: in particular, there is little hope of deriving these functions or relationships from simpler existing laws. Our Conjecturing framework aims to help fill this gap in current capabilities.

3.1. Discovering Gravity

In this example, a numeric invariant of interest is determined by a more complex nonlinear relationship with three numeric predictors. Consider measurements including the masses of two objects m_1 and m_2 , their distance r, and the gravitational force between them F. The goal is to recover the dependence of F on m_1 , m_2 , and r, or

$$F = k \frac{m_1 m_2}{r^2},$$

where k is the gravitational constant. Following the demonstration by Langely et al. (1987), we create a fictional dataset using a predefined value for k that is a random number between 0 and 1. For our illustrative example, we generated 1,000 training data points and 1,000 test data points with k = 0.057098. Values for m_1 , m_2 , and r are samples from Uniform(1,100000) distributions, and F is calculated for each sample with no noise.

A linear regression model will fail to capture the nonlinear interaction of the variables. Offthe-shelf machine learning methods such as random forests and neural networks can leverage the nonlinear relationship in the data but cannot present the relationship to the investigator. In the next section, we propose a framework for producing bounds on F that are functions of the other features.

3.2. Discovering an Interaction in Real Estate Valuation Data

The second example is a case where a boolean variable of interest is completely determined by the product of two numeric features in the dataset; i.e., the second-order *interaction* term completely defines the relationship.

Consider a dataset on residential real estate properties for sale obtained from https://www.redfin.com. The goal is to predict whether a home with given feature values has a list price above or below \$300,000.

This dataset includes both the price per square foot and total square footage along with eight additional features such as the number of bathrooms and bedrooms. The property of interest (above vs. below) can be determined by multiplying the price per square foot by square footage and setting a threshold. Thus, the interaction of price per square foot and square footage, hereafter called the *active interaction*, completely describes the relationship between the predictors and response. Data are partitioned into a training dataset with 1,000 houses and a test dataset with 30,156 houses. In the next section, we leverage our framework for invariant bounds and then extend it to produce boolean relationships to recover the active interaction term and how it determines class membership.

4. A Conjecturing Framework for Discovering Patterns in Data

We now describe a framework that leverages a conjecturing algorithm to discover nonlinear and boolean feature relationships in data. All experiments were run on a computer with an Intel i7-2600 CPU @ 3.4GHz and 16 GB RAM.

4.1. Conjecturing for Nonlinear Relationships

The invariant version of the conjecturing method (**procedure** Conjecturing-INV) can be used for discovering nonlinear relationships in data. Invariant conjectures are generated that provide upper and lower bounds on the invariant of interest. These conjectures are the nonlinear functions that can be used as new features and/or as a complete model for the system.

For the gravity case from Section 3.1, the invariants are $A = \{F, m_1, m_2, r\}$ and the invariant of interest is the force F. The examples E are the observations in the data.

The Conjecturing framework is not designed to recover constants such as the gravitational constant k. In general, for a functional relationship with a constant k such that 0 < k < 1, the

expression without the constant provides a lower bound for the response and the reciprocal expression provides an upper bound. In cases where the constant is not between 0 and 1, the converse is true. For this example, $F = km_1m_2/r^2$ with 0 < k < 1 and so $r^2/m_1m_2 \le F \le m_1m_2/r^2$. The Conjecturing framework can potentially recover the bounds $F \le m_1m_2/r^2$ or $F \ge r^2/m_1m_2$.

For our example, Conjecturing-INV returns 19 upper bounds and 24 lower bounds for F. Among the upper bounds is

$$F \le m_1 m_2 / r^2,$$

which approximates the true gravity relationship used to generate the data. The bound does not include the constant k. The lower bound of r^2/m_1m_2 is not recovered. Other bounds generated by Conjecturing-INV include

$$F \le 2m_2/\sqrt{r},\tag{1}$$

$$F \le 2|m_1 - m_2|,\tag{2}$$

$$F \ge 8m_2/r^2,\tag{3}$$

$$F \ge -1/(r - 2m_2). \tag{4}$$

Eight of the upper bounds and 15 of lower bounds for F are depicted in Figure 2. The upper bound m_1m_2/r^2 in Figure 2(a) is blue, while the true value km_1m_2/r^2 is gold.

As the primary goal of our approach is discovery, the bounds produced are suggestions that require further validation. We consider it a success that the relationship $F \propto m_1 m_2/r^2$ is included in one of the bounds. Among the other bounds produced, we see that true relationships $F \propto m_1$, $F \propto m_2$, and $F \propto 1/r^2$ are all suggested, along with false relationships $F \propto 1/\sqrt{r}$ and $F \propto 1/r$. Follow up investigations can be used to inspect these relationships and potentially recover the gravitational constant. The lower bound that is not recovered, while valid, does not reflect the true proportionality relationships which may be why it is dominated by other bounds. An approximation of the gravitational constant of 0.057 could be represented as $(+1+1+1+1+1) \times 10^{-1-1} + (+1+1+1+1+1) \times 10^{-1-1-1}$ which by itself has complexity 19. The expression $m_1 m_2/r^2$ has complexity 6.

In this example, the CONJECTURING framework recovers the true nonlinear relationship up to a constant of proportionality along with 44 additional suggested bounds. Therefore, isolating a single true bound, in the case where the bound is unknown, can require additional analysis and/or experiments. The additional bounds can provide potential insight into feature interactions.

4.2. Conjecturing for Nonlinear and Boolean Relationships with Mixed Data

Our Conjecturing framework for mixed data leverages the invariant version (**procedure** Conjecturing-INV) and the property version (**procedure** Conjecturing-PROP) of the conjecturing algorithm. For mixed data, we propose a framework to produce conjectures of nonlinear and boolean patterns. These conjectures can capture complex patterns while maintaining interpretability.

We assume that we are given a dataset with numeric features N, boolean features B, and a categorical feature of interest with levels \mathcal{Y} . Note that a categorical feature with more than two levels can be converted to a series of boolean features. Let π_y be the property that an observation has value y, for $y \in \mathcal{Y}$.

For each level $y \in \mathcal{Y}$, the algorithm discovers bounds for the numeric features that are satisfied by each observation in the class (Algorithm 2, Lines 4-14). These inequalities are converted to properties of the form "if the inequality is satisfied, then true; false, otherwise" (Algorithm 2, Line 12). These new properties are combined with the original boolean features in the data (Algorithm 2, Line 13). The properties from across all classes are pooled together and the observations belonging to all classes are pooled together as examples and then, for each level $y \in \mathcal{Y}$, the property version of conjecturing is applied to discover sufficient conditions for π_y (Algorithm 2, Lines 15-20).

We now provide further details on Algorithm 2 using the real estate valuation case from Section 3.2 as an illustrative example. First, we convert the categorical feature propertyType into boolean features condo, mobileHome, singleFamily, townhouse, multiFamily2-4Unit, multiFamily5PlusUnit, and Other. We also add a feature that is a constant value of 300,000 for each observation because it is the price cutoff and call it 300K. The resulting 18 features are partitioned into numeric features $N = \{bedrooms, bathrooms, squareFootage, lotSize, yearBuilt, daysOnMarket, pricePerSquareFoot, <math>hoaPerMonth$, latitude, longitude, longi

In our training set, there are 1,000 observations that are used as examples. For each value of the property of interest, {below, above}, the corresponding observations serve as the examples (Algorithm 2, Line 6). For each numeric feature, upper and lower bounds on that feature are found that are functions of the other numeric features (Algorithm 2, Lines 8-9). These are found by applying the invariant relations version of the conjecturing method (Conjecturing-INV). For houses with property below, there are 1,280 bounds derived. Included are plausible relations concerning house features that are seemingly irrelevant to the classification task such as

$$bathrooms \le 2 \times bedrooms \tag{5}$$

$$bedrooms \ge bathrooms - 1$$
 (6)

$$lotSize \ge (squareFootage - yearBuilt) \times bedrooms \tag{7}$$

Also included are less-interpretable bounds such as:

$$yearBuilt \ge hoaPerMonth \times \log(10)/\log(2 \times daysOnMarket)$$
 (8)

$$daysOnMarket \le e^{e^{\sqrt{2 \times lotSize}}} \tag{9}$$

$$hoaPerMonth \le 10^{2 \times bathrooms} + squareFootage$$
 (10)

There were also several bounds discovered that are close approximations of the relationship present in the active interaction term, including

$$squareFootage \le 300K/pricePerSquareFoot + bathrooms$$
 (11)

$$squareFootage \le 300K/pricePerSquareFoot + bedrooms$$
 (12)

$$squareFootage \le 300K/pricePerSquareFoot + daysOnMarket$$
 (13)

$$squareFootage \le 300K/(pricePerSquareFoot-1)-1$$
 (14)

$$pricePerSquareFoot \le -300K/(bedrooms - squareFootage)$$
 (15)

$$pricePerSquareFoot \le \lceil 300K/squareFootage \rceil$$
 (16)

$$300K \ge -(bathrooms - squareFootage) \times pricePerSquareFoot$$
 (17)

For houses with property *above*, there are 1,457 bounds derived including a mix of simple relations and less intuitive relations. Also included are the following three relations that are nearly identical to the active interaction relation:

$$squareFootage \ge 300K/(pricePerSquareFoot+1)$$
 (18)

$$price Per Square Foot \ge 300 K/square Footage + 1$$
 (19)

$$300K \le (pricePerSquareFoot+1) \times squareFootage$$
 (20)

The resulting invariant relations are pooled together (Algorithm 2, Line 10). The invariant relations are encoded as properties (Algorithm 2, Line 12). The original binary features from the

data are also encoded as properties for a total of 1,280 + 1,457 + 7 = 2,744 properties. Examples of encoded properties from the invariant relations are:

$$bathrooms \stackrel{?}{\leq} 2 \times bedrooms$$
 (21)

$$(yearBuilt \stackrel{?}{\geq} hoaPerMonth \times \log(10) / \log(2 \times daysOnMarket))$$
 (22)

$$(squareFootage \stackrel{?}{\leq} 300K/pricePerSquareFoot + bathrooms) \tag{23}$$

$$(squareFootage \stackrel{?}{\geq} 300K/(pricePerSquareFoot+1)).$$
 (24)

These properties can be used as boolean features that indicate whether a nonlinear relationship among numeric features is satisfied for an observation.

The properties generated for each level $\{below, above\}$ are collected in a set Π along with π_y and the seven original boolean features (Algorithm 2, Line 13).

For each level $\{below, above\}$, apply the property version of conjecturing to the properties Π with the training data observations serving as the examples E and level as the property of interest (Algorithm 2, Lines 15-20). The result is a set of properties that are sufficient conditions for the levels.

Conjecturing-Properties only two properties. They both approximate the underlying active interaction.

$$bathrooms \ge -300 K/pricePerSquareFoot + squareFootage \qquad \rightarrow isBelow \qquad (25)$$

$$squareFootage \ge (300K+1)/(pricePerSquareFoot-1)$$
 $\rightarrow isAbove$ (26)

An inspection of the data reveals that for some of the houses, there is some rounding error when comparing the price to the square footage multiplied by the price per square foot. The conjecturing algorithm compensates by using invariants as error terms. In the first property, the error term is $bathrooms \times pricePerSquareFoot$. In the second property, the error term is squareFootage + 1.

When these properties are applied as classification rules for predicting whether a house will be above or below \$300,000, they produce no error on the training data. The first property misclassifies 37 of 30,156 houses in the test data for an accuracy of 0.999. The second property misclassifies 26 houses. The misclassified houses are due to rounding error and miscoding of data. For example, one house in the test data is listed as having 31,248 bathrooms and another is listed as having a price of \$459.

Despite the noise and rounding error in the data, the CONJECTURING framework was able to recover the active interaction term and these properties can be used as features for classifiers with near-perfect accuracy.

Hereafter, we use "Conjecturing framework" to imply:

Algorithm 2 Conjecturing framework for nonlinear and boolean relationships with mixed data Input: Data observations $\{1, ..., n\}$ with numeric features N, boolean features B, and a categorical feature of interest with levels \mathcal{Y} ; a set of invariant operators O and a set of property operators P. Output: A set of conjectured properties \mathcal{P} .

```
1: Set \mathcal{P} = \emptyset. /* Initialize properties set. */
```

- 2: Set $A = \{\alpha_j : j \in N\}$. /* Define the set of invariants to be the original numeric features in the data. */
- 3: Set $\Pi = \{\pi_j : j \in B\}$. /* Define the set of properties to be the original boolean features in the data. */
- 4: for $y \in \mathcal{Y}$ do /* Loop on the levels of the categorical feature of interest. */
- 5: Set $\mathcal{R} = \emptyset$. /* Initialize invariant relations set. */
- 6: Set $E = \{i : \pi_y\}$. /* Define the set of observations with level y as the examples. */
- 7: **for** $j \in N$ **do** /* Loop on original numeric features. */
- 8: Set $R_U = \text{Conjecutring-INV}(E, A, O, \alpha_j, UPPER)$ /* Submit examples, invariants, and the invariant of interest to the invariant version of Conjecturing for upper bounds. */
- 9: Set $R_L = \text{Conjecturing-INV}(E, A, O, \alpha_j, LOWER)$ /* Submit examples, invariants, and the invariant of interest to the invariant version of Conjecturing for lower bounds. */
- 10: Set $\mathcal{R} = \mathcal{R} \cup R_U \cup R_L$.
- 11: end for
- 12: Convert the new invariant relations \mathcal{R} into properties $\Pi_{\mathcal{R}}$.
- 13: Set $\Pi = \Pi \cup \pi_y \cup \Pi_{\mathcal{R}}$. /* Define the set of properties to be the original boolean features, the level y, and the invariant relations properties. */
- 14: end for
- 15: for $y \in \mathcal{Y}$ do /* Loop again on the levels of the categorical feature of interest. */
- 16: Set $E = \{1, \dots, n\}$. /* Use all examples. */
- 17: Set $\mathcal{P}_S = \text{Conjecturing-PROP}(E, \Pi, P, \pi_y, SUFFICIENT)$. /* Submit examples, properties, and the level y as the property of interest to the property version of Conjecturing for sufficient conditions. */
- 18: Set $\mathcal{P}_N = \text{Conjecturing-PROP}(E, \Pi, P, \pi_y, NECESSARY)$. /* Submit examples, properties, and the level y as the property of interest to the property version of Conjecturing for necessary conditions. */
- 19: Set $\mathcal{P} = \mathcal{P} \cup \mathcal{P}_S \cup \mathcal{P}_N$.
- 20: **end for**
- 21: return \mathcal{P} .

- 1. In the case that all features are numeric, apply **procedure** Conjecturing-INV.
- 2. In the case that all features are categorical, convert the features to a series of properties (boolean features) and apply **procedure** Conjecturing-PROP.
 - 3. In the case of mixed data, apply Algorithm 2.

If there is no invariant of interest or no property of interest, each invariant and/or property can serve as the invariant/property of interest in turn, and conjectures can be generated for each.

5. Additional Computational Experiments

5.1. Sensitivity to the Number of Features

To investigate the impact of the number of features on the performance on the Conjecturing framework, we conduct experiments adding noisy features to the gravity example. We use the same experimental setup as described in Section 4.1 including a time limit of five seconds. For k = 0, ..., 10, we add k noise invariants generated from a standard normal distribution and check 1) whether Conjecturing-INV recovers $m_1 m_2/r^2$, 2) the number of conjectures produced, 3) the number of expressions evaluated, and 4) the number of valid expressions produced. Valid expressions are bounds that are valid for all training examples.

For k = 0, ..., 6, Conjecturing-INV recovers $m_1 m_2/r^2$ as a conjectured upper bound and for k = 7, ..., 10 the bound is not recovered because of the additional noise invariants. The number of original invariants is five including the force F, so in this experiment we can add more than 100% additional invariants and still recover the true proportionality relationship $F \propto m_1 m_2/r^2$.

Figure 4 contains plots of the number of conjectures produced, number of expressions evaluated, and the number of valid expressions produced within the five second time limit. The number of conjectures produced and expressions evaluated increases as the number of columns increases and tends to be larger for lower bounds than upper bounds. The number of conjectures produced ranges from 22 to 174. The number of valid expressions fluctuates between 75,000 and 135,000 and there is no discernible pattern effect of the number of noise invariants k. As k increases, there are more invariants available and the number of low-complexity expressions increases exponentially as does the number of low-complexity expressions comprised of the noise invariants. Low-complexity expressions can be generated and checked more quickly which is why the number of expressions evaluated increases with k. The number of expressions evaluated in five seconds ranges between about 300,000 and 1.4 million.

5.2. Sensitivity to Training Examples

To investigate the effect of different subsets of training examples on the ability of the Conjectur-ING framework to recover true relationships, we apply the framework to the real estate experiment

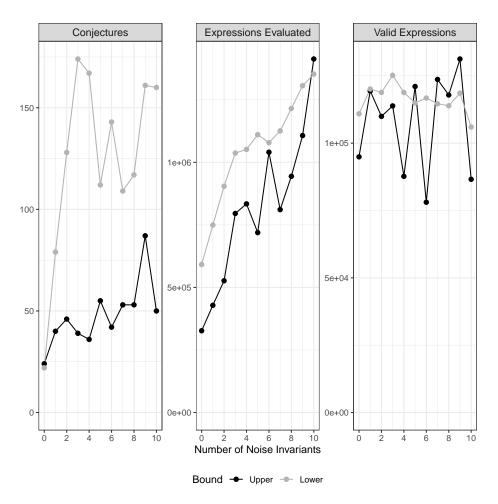


Figure 4 The number of conjectures produced, expressions tested, and valid experessions produced as a function of the number of noise invariants added to the gravity experiment.

with 10 random samples of 1,000 training examples. We use the same experimental setup as described in Section 2 including a time limit of five seconds.

Table 1 contains the conjectures produced by the Conjecturing framework for each of the 10 replications. As in the experiment in Section 4.2, the Conjecturing framework makes use of invariants and operators to compensate for rounding error. The invariants employed as tolerances are bathrooms and longitude. The framework also employs operators +1, -1, and $\lceil \cdot \rceil$ to account for deviations from the underlying active interaction. Each of the bounds can be rewritten in terms of squareFootage \times pricePerSquareFoot -300K plus or minus a small error term containing at most one additional invariant. Therefore, we see that in this instance, the method is not sensitive to the choice of training examples. Further experiments are needed to understand how well the Conjecturing framework can recover underlying relationships in the presence of different kinds of noise. This is the subject of future work.

Table 1 Sufficient Conditions Produced by Conjecturing for Different Training Set Samples for the Real Estate

Valuation Data

Sample	Conjectures Produced
1	$bathrooms \ge -300K/pricePerSquareFoot + squareFootage \rightarrow isBelow$
	$squareFootage \ge (300K+1)/(pricePerSquareFoot-1)) \rightarrow isAbove$
2	$squareFootage \leq \lceil 300K/pricePerSquareFoot \rceil \rightarrow isBelow$
	$ squareFootage \ge (300K+1)/(pricePerSquareFoot-1) \rightarrow isAbove$
3	$bathrooms \ge -300 K/pricePerSquareFoot + squareFootage \rightarrow isBelow$
	$ squareFootage \ge (300K+1)/(pricePerSquareFoot-1)) \rightarrow isAbove$
4	$bathrooms \ge -300 K/pricePerSquareFoot + squareFootage \rightarrow isBelow$
	$ squareFootage \ge (300K+1)/(pricePerSquareFoot-1)) \rightarrow isAbove$
5	$bathrooms \ge -300 K/pricePerSquareFoot + squareFootage \rightarrow isBelow$
	$ squareFootage \ge (300K+1)/(pricePerSquareFoot-1)) \rightarrow isAbove$
6	$ squareFootage \le \lceil 300K/pricePerSquareFoot \rceil \rightarrow isBelow$
	$squareFootage \ge (300K+1)/(pricePerSquareFoot-1) \rightarrow isAbove$
7	$ squareFootage \le (300K + longitude)/pricePerSquareFoot \rightarrow isBelow$
	$squareFootage \ge (300K+1)/(pricePerSquareFoot-1)) \rightarrow isAbove$
8	$bathrooms \ge -300 K/pricePerSquareFoot + squareFootage \rightarrow isBelow$
	$squareFootage \ge (300K+1)/(pricePerSquareFoot-1)) \rightarrow isAbove$
9	$ squareFootage \le (300K - daysOnMarket)/pricePerSquareFoot \rightarrow isBelow$
	$squareFootage \ge (300K+1)/(pricePerSquareFoot-1) \rightarrow isAbove$
10	$bathrooms \ge -300 K/pricePerSquareFoot + squareFootage \rightarrow isBelow$
	$squareFootage \ge (300K+1)/(pricePerSquareFoot-1)) \rightarrow isAbove$

5.3. Comparison to AI Feynman (Udrescu and Tegmark 2020)

In this section, we compare the ability of Conjecturing to recover equations from datasets used by Udrescu and Tegmark (2020) with their algorithm AI Feynman. We then apply the implementation of AI Feynman to the gravity and real estate datasets described in Section 3. We note that the primary goal of Conjecturing is for discovery of nonlinear and boolean relationships while the primary goal of AI Feynman is recovery of equations.

Performance on Feynman Equations. We apply Conjecturing to the first 10 equations listed in Table 4 of (Udrescu and Tegmark 2020) to draw comparisons based on solution time and noise tolerance. We used the data published by the authors here: https://space.mit.edu/home/tegmark/aifeynman.html. As in (Udrescu and Tegmark 2020), for each instance we apply Conjecturing with three subsets of operators in turn: $\{+,-,\times,\div,+1,-1,^2,\sqrt\}$, $\{+,-,\times,\div,+1,-1,^2,\sqrt,\sin,\cos,\ln,^{-1},e\}$, $\{+,-,\times,\div,+1,-1,^2,\sqrt,\sin,\cos,\ln,^{-1},e,|\cdot|,\sin^{-1},\tan^{-1}\}$. For instances where an equation includes the constant π , we include π as a constant invariant. For each instance, we use the first 10 samples in each dataset and run Conjecturing for 10, 100, and 1,000 seconds. We also run Conjecturing for the noise tolerance of and time required by AI Feynman to recover the equations as reported in Table 4 of (Udrescu and Tegmark 2020).

Tables 2 and 6 contain the results of applying Conjecturing to the datasets. Conjecturing produces bounds that match the equation for four of the ten instances. Conjecturing finds a match for all equations with complexity 10 or less and is unable to find a match for equations with higher complexity. Udrescu and Tegmark (2020) report that AI Feynman resolves all of the equations while Eureqa (Schmidt and Lipson 2009) resolves four of the ten equations, three of which are different from those found by Conjecturing. These results indicate that Conjecturing is well suited for recovering equations of complexity 10 or less within 1,000 seconds and sometimes within much shorter times. Higher-complexity formulas with more invariants require additional time.

Equations I.6.2 and I.6.2.b in Table 2 each have a repeated invariant σ . As noted in Section 2.2, Conjecturing does not allow repeated invariants and so these equations will not be recoverable as bounds. In Section 5.4, we describe ways to address this deficiency and recover equations such as I.6.2 and I.6.2.b.

The normalized root-mean-square error (NRMSE) calculated for 100 test examples for the bestperforming conjecture on the training data based on mean absolute error. NRMSE is calculated as $1/\sigma_f$ multiplied by the root-mean-square error on the test examples, where σ_f is the standard deviation of the invariant of interest for the test examples. Conjecturing produced conjectures with NRMSE less than 1.0 for 7 of the 10 equations.

Despite the fact that Conjecturing is not designed for recovery of equations, we see that it can be successful in doing so for lower-complexity, albeit nonlinear, equations.

Table 6 in the Appendix contains the results of applying Conjecturing to the datasets when noise is added to the invariant of interest. The noise in the table is the standard deviation of the normal distribution with mean zero added to the invariant of interest; the noise is the noise level tolerated by AI Feynman as reported by Udrescu and Tegmark (2020). The time is the time reported by Udrescu and Tegmark (2020) for AI Feynman to recover the equation.

Conjecturing is unable to achieve exact recovery of the equations with the introduction of noise. The NRMSE is less than 1.0 for six of the 10 equations and does not exceed 1.625. The strict requirements of the Dalmatian heuristic seem to prevent exact recovery in the presence of noise, but Conjecturing is still able to produce good approximations of the equations.

Performance of AI Feynman (Udrescu and Tegmark 2020) on Gravity and Real Estate Examples. We apply the implementation of AI FEYNMAN available here: https://github.com/SJ001/AI-Feynman to the gravity example described in Section 3.1 and the real estate example described in Section 3.2. A difference between our gravity example and the datasets used by Udrescu and Tegmark (2020) is that for the gravity example, the gravitational constant

Number of Recovered Instance Equation Invariants Complexity Time (s) NRMSEby Eureqa? $f = e^{-\theta^2/2} / \sqrt{2\pi}$ 10^{3} I.6.2.a 9 No 0.000 $f = e^{-\theta^2/2\sigma^2} / \sqrt{2\pi\sigma^2}$ 3 1.6.213 NA 0.553 No $f = e^{-(\theta - \theta_1)^2/2\sigma^2} / \sqrt{2\pi\sigma^2}$ I.6.2.b5 16 NA 1.092 No $d = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$ 10^{3} I.8.144 10 0.000No $\frac{Gm_1m_2}{(x_2-x_1)^2+(y_2-y_1)^2+(z_2-z_1)^2}$ I.9.189 17 NA 1.100 No I.10.73 9 5 0.000No 6 NA Yes I.11.19 $A = x_1 y_1 + x_2 y_2 + x_3 y_3$ 11 1.014 I.12.1 $F = \mu N_n$ 2 Yes 3 5 0.000 $F = \frac{q_1 q_2}{4\pi \epsilon r^2}$ $F = -\frac{q_1}{q_1}$ I.12.25 12 NA 0.671Yes I.12.44 NA 0.135Yes 11

Table 2 Results for Conjecturing on Datasets from (Udrescu and Tegmark 2020)

G is the same for every data point, but for the datasets used by Udrescu and Tegmark (2020), G is treated as a variable and is different for each point.

For the real estate data, we apply AI FEYNMAN to the data to attempt to discover the relationship between the property of interest and the input features. The original numeric features are supplied along with boolean features corresponding to the levels of the *propertyType* feature. Note that AI FEYNMAN is designed for recovering numeric functions and is therefore not suitable for boolean relationships such as those in the real estate example.

For both instances, the AI FEYNMAN implementation aborts with an error regarding an eigenvalue calculation. We suspect that the source of the failure in both cases may be due to the difference in treatment of constants. In our gravity example, the gravitational constant is the same for all points while in analogous examples, Udrescu and Tegmark (2020) treat constants as variables and generate a unique value for each observation. Our practice of treating the gravitational constant as the same for all observations may be contributing to an error in matrix calculations for AI FEYNMAN. In the real estate example, each observation has a feature with the same value (the \$300,000 cutoff). This constant column in the data matrix could also be contributing to an error in matrix calculations for AI FEYNMAN. In the electronic companion, we include the code and output for AI FEYNMAN applied to 1) their Example 1, demonstrating that our installation is functional, 2) our gravity example, including the error message, and 3) our real estate example, including the error message, These examples show that the Conjecturing framework can provide useful insights on examples where AI FEYNMAN cannot.

5.4. Experiments with the Nguyen Benchmark Suite Nguyen et al. (2011)

We apply our invariant conjecturing implementation to the Nguyen benchmark suite (Nguyen et al. 2011) so as to draw comparisons with symbolic regression methods described by Petersen et al. (2021). The Nguyen benchmark suite is a set of 12 equations. As mentioned before, our Conjecturing framework is designed for discovering nonlinear relationships in the form of bounds

and boolean relationships while symbolic regression methods are designed to recover equations. In these experiments, we investigate the ability of invariant conjecturing to recover equations (or approximations) among the discovered bounds.

The benchmark equations are in Table 3. We generate an instance for each using the protocols described by Petersen et al. (2021). For each equation, 20 training examples and 20 test examples are generated. For equations 1 though 6, x is sampled from a Uniform(-1,1) distribution; for equation 7, x is sampled from a Uniform(0,2) distribution; for equation 8, x is sampled from a Uniform(0,4) distribution; for equations 9 through 12, x and y are sampled from a Uniform(0,1) distribution. For each equation, we allow a time limit of 10,000 seconds for generating upper and lower bounds. The operators include unary operators sine, cosine, natural log, and natural exponential, and binary operators addition, subtraction, multiplication, and division.

As noted in Section 2.2, our CONJECTURING framework does not allow repeated invariants in conjectures. Therefore, most of the equations in Table 3 cannot be recovered by our framework. For each equation, we first evaluate the ability of the conjectured bounds to approximate the equation by reporting the normalized root mean squared error (NRMSE) as defined and reported by Petersen et al. (2021) and described in Section 5.3. We report NRMSE for the conjecture with the lowest mean average error for the training examples.

The results in Table 3 indicate that our Conjecturing framework is able to recover only equation $11 \ f = x^y$. It is able to do so despite the fact that the exponent operator is not included. Conjecturing produces the expression $e^{y\log(x)}$ and simplified it to x^y . The NRMSE values for the best bounds for the other instances range from 0.22 to 1.08. These values are larger than those reported for symbolic regression methods as reported in Table 10 of Petersen et al. (2021); the methods include deep symbolic regression (DSR) Petersen et al. (2021), priority queue training (PQT) Abolafia et al. (2018), vanilla policy gradient (VPG) Petersen et al. (2021), genetic programming (GP), and a method implemented in Mathematica based on Markov chain Monte Carlo and nonlinear regression.

For expressions 1 through 8, the only invariants are the invariant of interest f and the input invariant x. Because of the fact that no invariants can be repeated, the Conjecturing framework is limited to the application of only unary operators to x and no expressions with binary operators are produced. As an example, for the first equation, the best conjectured lower bound is

$$f(x) \ge \sin(e^{e^{\cos(\sin(\sin(\sin(\sin(\sin(\sin(\sin(\cos(\cos(\sin(e^x))))))))))}}).$$

We now describe how our CONJECTURING framework can be adapted to allow for repeated invariants, and report results for the adapted method. To address repeated invariants, we can add

		Without Add	litional Invariants	With Additio	nal Invariants
Instance	Equation	Recovered?	NRMSE	Recovered?	NRMSE
1	$f = x^3 + x^2 + x$	No	0.94	Yes	0.00
2	$f = x^4 + x^3 + x^2 + x$	No	0.86	Yes	0.00
3	$f = x^5 + x^4 + x^3 + x^2 + x$	No	1.01	Yes	0.00
4	$f = x^6 + x^5 + x^4 + x^3 + x^2 + x$	No	0.63	Yes	0.00
5	$f = \sin\left(x^2\right)\cos\left(x\right) - 1$	No	0.22	Yes	0.00
6	$f = \sin\left(x\right) + \sin\left(x + x^2\right)$	No	0.44	Yes	0.00
7	$f = \log(x+1) + \log(x^2 + 1)$	No	0.58	Yes	0.00
8	$f = \sqrt{x}$	No	1.08	Yes	0.00
9	$f = \sin\left(x\right) + \sin\left(y^2\right)$	No	1.03	Yes	0.00
10	$f = 2\sin(x)\cos(y)$	No	0.60	Yes	0.00
11	$f = x^y$	Yes	0.00	Yes	0.00
12	$f = x^4 - x^3 + \frac{1}{2}y^2 - y$	No	0.83	Yes	0.00

Table 3 Results for Conjecturing on the Nguyen Benchmark Suite Nguyen et al. (2011)

additional invariants using commonly-occurring functional forms. For equations 1 through 8, we add invariants x^2 , x^3 , x^4 , x^5 , x^6 , $\sin(x)$, $\cos(x)$, \sqrt{x} along with two copies of the constant 1, and the constant 2. Two copies of the constant 1 are included because it appears twice in equation 7. For equations 9 through 12 we also add y^2 as an invariant. Recall that in our implementation, while invariants cannot repeat in a conjectures, operators can. Therefore, an alternative approach to addressing the constants is to include the unary operator of addition by 1.

As shown in Table 3, the Conjecturing framework is able to exactly recover each equation as a bound when the additional invariants are included so that the NRMSE values are 0.000 for all equations.

The practice of adding the invariants that are nonlinear functions of the original input might appear to be impractical. However, as suggested by Brunton et al. (2016), specifying these invariants can reflect expert knowledge on the system being investigated. They note that identifying candidate functions for SINDy "must be a coordinated effort to incorporate expert knowledge, feature extraction, and other advanced methods." Conjecturing offers distinct capabilities for discovery, as nonlinear functions can be specified as invariants or may still be discovered so long as they do not involve repeated input invariants.

6. Application to COVID-19 Data

In this section, we demonstrate the Conjecturing framework on synthetic patient-level COVID-19 data that was provided as part of the Veterans Health Administration (VHA) Innovation Ecosystem and precisionFDA COVID-19 Risk Factor Modeling Challenge (https://precision.fda.gov/challenges/11/view). The data include synthetic veteran patient health records including medical encounters, conditions, medications, and procedures. All subjects are located in Massachusetts.

The goal of the challenge was to better understand risk and protective factors for COVID-19 outcomes. Participants were asked to predict alive/deceased status. Since our goal is to discover potential risk and protective factors, we evaluate the performance of CONJECTURING by checking the performance of the feature relationships on holdout test data rather than on prediction accuracy. Establishing the risk and protective factors as causal would require additional controlled experiments.

Predictions were based on information obtained through December 31, 2019. In the training data, we drop all information pertaining to events on or after January 1, 2020 and drop subjects who died before January 1, 2020.

We add a number of features for each patient based on the data, described in Table 7 in the Appendix. In addition, for each numeric observation, we created invariants for the mean and most recent value and for each reported allergy, device, immunization, procedure, and discretely-measured observation we create a property corresponding to each level. In total, we use 309 invariants and 362 properties. We use a training set consisting of 100 subjects from each outcome class (deceased/alive). We compare the results of applying Conjecturing with classification and regression trees (CART) Breiman et al. (1984) which is another interpretable method.

6.1. Results for Conjecturing

Upper and lower bounds are generated for each invariant, and for each outcome. These bounds, along with the 362 properties in the data, are used as properties for Conjecturing-PROP. Conjectures are generated for both outcomes. The parameter *skips* is set to 90%. We use the remaining 73,497 subjects as a test data set thereby allowing us to ascertain the effects of potential overfitting to the 200 subjects used for training.

Among those with COVID-19 in the test data, 5,468 (8.0%) have a status of deceased, and 68,029 (92.0%) are alive. There are 38 conjectures for sufficient conditions for alive status and 40 conjectures for sufficient conditions for deceased status produced by the framework. Tables 8-11 in the Appendix contain the conjectures and evaluations.

Tables 9 and 11 in the Appendix contain quantitative evaluations of the performance of the conjectures. Each table contains the precision, support, and lift of each conjecture. Note that each conjecture is a sufficient condition expressed as a conditional statement. The precision is the percentage of test examples for which the conditional statement evaluates to true among those for which the antecedent is true. Precision may be thought of as the "hit rate" of the conjecture. The support is the number of test examples for which the antecedent evaluates to true. The lift is the ratio of the precision to the proportion of examples for which the consequent is true. If the lift is greater than 1, then the conjecture is better at identifying people for which the consequent is true than a random selection from the population.

Of the 38 conjectures for alive status, 22 (57.9%) have lift at least 1.00. The lift ranges from 0.81 to 1.07; note that the maximum possible lift for a conjecture for alive status is 1.08 (1/(68029/73497)). Of the 40 conjectures for deceased status, 34 (85%) have lift at least 1.00. The lift ranges from 0.17 to 4.15.

Consider the sufficient conditions for deceased status in Table 10 in the Appendix. The conjecture with the highest precision and lift is

$$longitude > -age \times medicationsLifetimePercCovered \rightarrow Deceased,$$

and has a lift of 4.15 meaning that a subject for which $longitude > -age \times medications Lifetime Perc Covered$ is 4.15 times as likely to die as a randomly selected subject. The conjecture indicates that subjects in the east who are older and have a larger percentage of medications covered by the payer are at higher risk of death. The presence of longitude in the conjecture could be an indication of higher risk in population centers in the east such as Boston. The percentage of medications covered by the VHA is higher for subjects with more preexisting conditions and for those with more expensive medications because there is a low copay annual cap (currently \$700³). Further, the conjecture produces a suggestion of a functional form for the relationship between these factors. The conjecture confirms the CDC guidance that older subjects and those with more preexisting conditions are a higher risk of death from Covid⁴.

The conjecture with the second-highest precision and lift is

$$medications Active > |hemoglobin A1cHemoglobin Total InBlood| \rightarrow Deceased$$

with a lift of 3.29. The condition includes the number of active medications and the ratio of hemoglobin A1c to total hemoglobin (an HbA1c test). The conjecture indicates that those with more active medications than the HbA1c percentage are at higher risk of death, which again agrees with the CDC guidance concerning preexisting conditions. Typical values for HbA1c for non-diabetic patients are below 5.7%, while diabetic subjects can have values between 6.5% and 10.0% ⁵. The number of active medications can indicate a larger number of preexisting conditions, and the conjecture suggests that for diabetic patients, those with additional conditions are at higher risk.

The conjecture with the third-highest precision and lift is

$$age > carbonDioxide \times |potassium| \rightarrow Deceased,$$

 $^{^3}$ https://www.va.gov/health-care/copay-rates/, accessed July 10th, 2022

 $^{^4}$ https://www.cdc.gov/coronavirus/2019-ncov/need-extra-precautions/people-with-medical-conditions.html, accessed July 10th, 2022

⁵ https://www.cdc.gov/diabetes/managing/managing-blood-sugar/a1c.html, accessed July 10th, 2022

n = 200

with a lift of 3.12. The conjecture suggests that older subjects with lower CO_2 levels and lower potassium are at higher risk of death. Lower CO_2 levels and abnormal potassium levels, particularly lower levels, has been independently studied and associated with COVID-19 morbidity and mortality (Hu et al. 2021, Noori et al. 2022). In addition to validating a role for these invariants, the conjecture suggests a potential nonlinear relationship among them.

For both outcomes, the Conjecturing framework is able to generate new sufficient conditions that are true for the respective outcome at higher rates than would be expected for a patient selected at random. These results indicate that the conjecturing process is capturing relationships that hold across the population and are not merely reflective of the 200 training samples. In other words, overtraining appears to be mitigated. The discovered relationships, and the direct and indirect relationships that they indicate among features, are validated by the medical literature and provide suggestions for deeper investigations into the functional form of the relationships and the extent of causality. The number of conjectures generated is not overwhelming for a human investigator to consider and further investigate.

6.2. Comparison with an Interpretable Model

We now consider the results of applying classification and regression trees (CART) (Breiman et al. 1984) to the COVID-19 data. A model is fit using the implementation in the R library rpart (Therneau and Atkinson 2019). The tree produced by rpart is

```
node), split, n, loss, yval, (yprob)
  * denotes terminal node
```

- 1) root 200 100 False (0.50000000 0.50000000)
 - 2) age< 66.48323 92 17 False (0.81521739 0.18478261)
 - 4) active_care_plan_length< 33.3039 68 5 False (0.92647059 0.07352941) *
 - 5) active_care_plan_length>=33.3039 24 12 False (0.50000000 0.50000000)

 - 11) Body_Height< 167.15 16 5 True (0.31250000 0.68750000) *
 - 3) age>=66.48323 108 25 True (0.23148148 0.76851852)

 - 7) mean_Potassium< 4.85 98 19 True (0.19387755 0.80612245) *

Nodes 4, 6, 7, 10, and 11, correspond to leaf nodes. Each leaf node corresponds to a sufficient condition for deceased status (True) or alive status (False). Nodes 4, 6, and 10 correspond to

sufficient conditions for alive status, and nodes 7 and 11 correspond to sufficient conditions for deceased status. Tables 4 and 5 contain the conditions and quantitative evaluations of the conditions produced by CART. When comparing the results with those of Conjecturing in Tables 8-11 in the Appendix, we note that CART

- 1. produces many fewer conditions (3 versus 38 for alive status, 2 versus 40 for deceased status),
- 2. produces conditions that are in conjunctive normal form where each clause consists of a single numeric bound while Conjecturing tends to leverage nonlinear relationships among invariants as the basis for conditions,
- 3. produces two conditions with much larger support in the test data than those produced by Conjecturing (node 4 has 36,531 and node 7 has 12,443),
- 4. produces only two conditions that have lift greater than 1.0 (node 4 has lift 1.06 and node 7 has lift 2.85), and
- 5. does not produce conditions with better precision or lift than the best conditions produced by Conjecturing.

We note that both CART and CONJECTURING are able to leverage categorical variables for conditions, though CART does not do so for this training set. An example of such a condition is conjecture 27 in Table 10 in the Appendix.

Similar to many decision tree frameworks, CART leverages univariate bounds as component properties in its invariant clauses. Conjecturing is unlikely to derive numeric bounds for individual features but instead produces more nonlinear relationships between invariants. Decision tree frameworks such as CART and Conjecturing are complementary approaches for discovery of patterns among numeric and categorical features, but we see that Conjecturing is capable of producing more complex yet interpretable relationships.

Table 4 Conditions from CART for Alive/Deceased Status Among Those with COVID

Node Number	Sufficient Condition
$\overline{4}$	$age < 66.48 \& activeCarePlanLength < 33.30 \rightarrow Alive$
6	$age \geq 66.48 \ \& \ meanPotassium \geq 4.85 \rightarrow Alive$
10	$age < 66.48 \ \& \ active Care Plan Length \geq 33.30 \ \& \ body Height \geq 167.15 \rightarrow A live$
7	$age \ge 66.48 \ \& \ meanPotassium < 4.85 \rightarrow Deceased$
11	$age < 66.48 \& active Care Plan Length \ge 33.30 \& body Height < 167.15 \rightarrow Deceased$

Node Number Consequent Precision Support Lift 4 Alive 98.28% 36531 1.06 6 Alive 81.69% 2070 0.88 10 Alive 91.57% 5371 0.99 7 Deceased 21.17% 12443 2.85 11 Deceased 5.37% 3746 0.72					
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	Node Number	Consequent	Precision	Support	Lift
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	Alive	98.28%	36531	1.06
7 Deceased 21.17% 12443 2.85	6	Alive	81.69%	2070	0.88
	10	Alive	91.57%	5371	0.99
11 Deceased 5.37% 3746 0.72	7	Deceased	21.17%	12443	2.85
	11	Deceased	5.37%	3746	0.72

Table 5 Evaluation of Conditions from CART Among Those with COVID

7. Conclusions

We have demonstrated that automated search for conjectured feature-relations can enhance existing learning algorithms. The discovery of these kinds of feature relationships can also initiate new collaboration with domain scientists and lead to new scientific knowledge.

Our Conjecturing framework was able to recover the functional form for gravity with only the measured force, masses, and distance. The framework also recovered a hidden interaction between price per square foot, square footage, and price in real estate data that leads to improved classification performance. Using synthetic patient-level COVID-19 data, the framework produced conjectures that provide insight into the risk of death.

The current version of Conjecturing requires that conjectures are true for every example. Future research will adjust the algorithm to better handle noisy data by generating conjectures that do not necessarily hold for all examples. If the handling of noise can be improved, then Conjecturing may be able to be adapted to support predictive modeling efforts.

If the Conjecturing framework can provide functional relationships without constants of proportionality, the constant can be determined using regression with the original data. Suppose that the Conjecturing framework indicates a relationship between the response y and predictors x of the form $y \leq b_1 f(x)$ for an unknown constant b_1 . A regression model can be fit of the form $\hat{y} = b_0 + b_1 f(x)$ using the data (x_i, y_i) , i = 1, ..., n. The best strategy for determining constants of proportionality is another avenue for future research.

Another area for potential research involves the so-called p >> n problem. That is, if the number of features is larger than the number of observations, then there are insufficient degrees of freedom to estimate a linear model with all p features or any more complex model. In such situations, feature and/or model selection tools are needed to search over potentially large model spaces. As desired model complexity increases (e.g. consideration of interaction terms), searching over such large model spaces can become computationally prohibitive. For instance, suppose an investigator seeks to identify a model by selecting the "best" subset from among 10 features and their associated 45 two-way interactions. In this example, simply considering models with only 10 variables requires searching over a model space larger than 2.9 billion. Future research will investigate the ability of the Conjecturing framework to simplify model spaces and hence, provide a mechanism for a more expeditious search of plausible models.

Appendix A: Additional Results for Conjecturing for Recovery of Equations

Table 6 Additional Results for Conjecturing on Datasets from (Udrescu and Tegmark 2020)

		Number of				
Instance	Equation	Invariants	Complexity	Noise	Time (s)	NRMSE
I.6.2.a	$f = e^{-\theta^2/2} / \sqrt{2\pi}$	2	9	10^{-2}	16	0.234
I.6.2	$f = e^{-\theta^2/2\sigma^2} / \sqrt{2\pi\sigma^2}$	3	13	10^{-4}	2992	0.873
I.6.2.b	$f = e^{-(\theta - \theta_1)^2/2\sigma^2} / \sqrt{2\pi\sigma^2}$	5	16	10^{-4}	4792	1.625
I.8.14	$d = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$	4	10	10^{-4}	544	1.402
I.9.18	$\frac{Gm_1m_2}{(x_2-x_1)^2+(y_2-y_1)^2+(z_2-z_1)^2}$	9	17	10^{-5}	5975	0.977
I.10.7	$m = \frac{m_0}{\sqrt{1 - \frac{v^2}{c^2}}}$	3	9	10^{-4}	14	0.004
	$\sqrt{1-\frac{v^2}{c^2}}$					
I.11.19	$A = x_1 y_1 + x_2 y_2 + x_3 y_3$	6	11	10^{-3}	184	1.076
I.12.1	$F = \mu N_n$	2	3	10^{-3}	12	0.001
I.12.2	$F = \frac{q_1 q_2}{4\pi \epsilon r^2}$	5	12	10^{-2}	17	0.746
I.12.4	$E_f = \frac{q_1}{4\pi\epsilon r^2}$	4	11	10^{-2}	12	1.040

Appendix B: Features Generated for COVID-19 Data

Table 7 Feature Definitions for COVID-19 Data				
Feature Name	Definition			
health care Expenses	The total lifetime cost of healthcare to the patient			
health care Coverage	The total lifetime cost of healthcare services that were cov-			
_	ered by payers			
latitude	Latitude of patient's home address			
longitude	Longitude of patient's home address			
age	Current age of patient			
numAllergies	Number of ongoing patient allergies			
active Care Plans	Number of current care plans			
lifetime Care Plans	Number of lifetime care plans			
active Care Plan Length	Length of time under current care plans			
lifetime Care Plan Length	Total lifetime length under care plans			
active Conditions	Number of current health conditions			
lifetime Conditions	Number of lifetime health conditions			
active Condition Length	Amount of time since current health condition(s) diagnosis			
lifetime Condition Length	Amount of time since first diagnosis of a health condition			
deviceLifetimeLength	Total length of time using a medical device (e.g. pacemaker)			
encounters Count	Total number of encounters with a healthcare professional			
encounters Lifetime Total Cost	Total lifetime cost of healthcare encounters			
encounters Lifetime Base Cost	Total lifetime cost of healthcare encounters, not including			
	any line item costs related to medications, immunizations,			
	procedures, or other services			
encounters Lifetime Payer Coverage	Total lifetime cost of healthcare encounters that were covered			
	by payers			
encounters Lifetime Perc Covered	Percentage of lifetime cost of healthcare encounters that were			
	covered by payer			
imaging Studies Lifetime	Number of lifetime imaging diagnostics (e.g. MRI) performed			
	on patient			
immunizations Lifetime	Number of lifetime immunizations received by patient			
immunizations Lifetime Cost	Total lifetime cost of all immunizations received by patient			
medications Lifetime	Number of lifetime medications prescribed			
medications Lifetime Cost	Total lifetime cost of medications			
medications Lifetime Perc Covered	Percentage of lifetime medication cost coverered by payer			
medications Lifetime Length	Total lifetime length on prescribed medications			
medications Lifetime Dispenses	Total lifetime number of prescription dispenses			
medications Active	Number of current prescriptions			
procedures Lifetime	Number of lifetime medical procedures (e.g. surgery) per-			
	formed on patient			
procedures Lifetime Cost	Total lifetime cost of all medical procedures performed on			
	patient			

Appendix C: Results for Conjecturing Applied to COVID Data

Table 8 Conjectures for Alive Status Among Those with COVID

	Conjecture
1	$active Condition Length > age^2/latitude \rightarrow Alive$
2	$medicationsLifetime < -immunizationsLifetimeCost + 2 \times proceduresLifetime \rightarrow Alive$
3	$medicationsActive < \min\{sodium, \lfloor QOLS \rfloor\} \rightarrow Alive$
4	$activeCarePlans < e^{medicationsLifetimePercCovered} - immunizationsLifetime ightarrow Alive$
5	$active Care Plan Length < 10^{encounters Lifetime Perc Covered} \times active Care Plans \rightarrow A live$
6	$lifetimeConditionLength > \sqrt{QALY}^{activeConditions} \rightarrow Alive$
7	$lifetimeCarePlans > encountersCount/2 \rightarrow Alive$
8	$lifetimeCarePlans > \min\{triglycerides, \lfloor lifetimeConditions \rfloor\} \rightarrow Alive$
9	$encountersCount > activeConditions + medicationsLifetimeCost + 1 \rightarrow Alive$
10	$diabetes \ \& \ latitude < \sqrt{totalCholesterol} + meanCarbonDioxide \rightarrow Alive$
11	$active Care Plans > medications Lifetime^{medications Lifetime Cost} \rightarrow A live$
12	$lifetimeCarePlans > \sqrt{enountersCount} + QOLS \rightarrow Alive$
13	$age < lifetimeConditions \times log(latitude) \rightarrow Alive$
14	
15	v (/ L)
16	
17	
18	$health care Coverage > lifetime Condition Length^2 / imaging Studies Lifetime \rightarrow A live$
19	
20	
21	
22	$latitude < \sqrt{encountersLifetimeTotalCost} - medicationsLifetime \rightarrow Alive$
23	
24	
25	
26	$carbon Dioxide > respiratory Rate \times \lfloor hemoglobin A1 c Hemoglobin Total In Blood \rfloor \rightarrow A live$
	$osteoporosis Disorder \ \& \ lifetime Care Plan Length < \min \{pain Severity, 2 \times active Care Plan Length\} \rightarrow A live - active Care Plan Length = A live - activ$
28	$healthcareCoverage < \sqrt{encountersLifetimePayerCoverage} \times medicationsLifetime ightarrow Alive$
29	
30	
$\frac{31}{32}$	$prediabetes \& meanDiastolicBloodPressure > \lfloor carbonDioxide \rfloor + meanHeartRate \rightarrow Alive$
33	
34	· · · · · · · · · · · · · · · · · · ·
$\frac{34}{35}$	
36	·
$\frac{30}{37}$	medication e Lifetime Perc Covered \ latitude \frac{1}{2} medication e Lifetime Discourse \ \ Alive
38	
-30	$nea_{initial}$ $e \cup overlay e > \frac{1}{2 \times encounters Lifetime Perc Covered} op Allive$

Table 9 Evaluation of Conjectures for Alive Status Among Those with COVID

ition of Conject	uics for Allv		nong i
Conjecture	Precision	Support	Lift
1	99.11%	3042	1.07
2	98.54%	3700	1.06
3	98.51%	9480	1.06
4	98.25%	8231	1.06
5	98.23%	6103	1.06
6	98.05%	7937	1.06
7	97.79%	4161	1.06
8	97.65%	5453	1.05
9	97.65%	2939	1.05
10	97.41%	1969	1.05
11	97.07%	4774	1.05
12	96.79%	2242	1.05
13	96.61%	1650	1.04
14	95.65%	2045	1.03
15	95.39%	6311	1.03
16	95.31%	1236	1.03
17	95.20%	1687	1.03
18	95.07%	4017	1.03
19	94.32%	440	1.02
20	94.00%	500	1.02
21	93.59%	1498	1.01
22	93.25%	1185	1.01
23	92.09%	834	0.99
24	91.01%	1213	0.98
25	90.79%	999	0.98
26	89.77%	831	0.97
27	89.41%	727	0.97
28	88.61%	2389	0.96
29	88.27%	358	0.95
30	88.21%	704	0.95
31	87.67%	1890	0.95
32	87.20%	2250	0.94
33	87.14%	583	0.94
34	85.79%	1612	0.93
35	84.50%	755	0.91
36	82.76%	586	0.89
37	76.22%	677	0.82
38	74.75%	99	0.81

Table 10 Conjectures for Deceased Status Among Those with COVID

Conjecture	Sufficient Condition
1	$longitude > -age \times medicationsLifetimePercCovered ightarrow Deceased$
2	$medicationsActive > hemoglobinA1cHemoglobinTotalInBlood \rightarrow Deceased$
3	$age > carbonDioxide imes \lfloor potassium \rfloor o Deceased$
4	$deviceLifetimeLength \leq 2 \times creatinine^{healthcareExpenses} \rightarrow Deceased$
5	implantable Cardiac Pacem ightarrow Deceased
6	$latitude < \log(age)/\log(10)^{activeCarePlans} \rightarrow Deceased$
7	$medications Active > \lceil \log(alkaline Phosphatase Enzymatic\ Activity) / \log(10) \rceil \rightarrow Deceased$
8	$immunizationsLifetimeCost < age \times immunizationsLifetime^2 \rightarrow Deceased$
9	$colonoscopy \ \& \ coronary Heart Disease \rightarrow Deceased$
10	$active Care Plans < \min \{ device Lifetime Length, medications Active \} \rightarrow Deceased$
11	$glucose > \lceil creatinine \times meanGlucose \rightarrow Deceased$
12	$bodyWeight > \lfloor meanBodyWeight \rfloor + 1 \rightarrow Deceased$
13	$health care Expenses < device Lifetime Length^2 \times lifetime Condition Length \rightarrow Deceased$
14	$lifetime Conditions > active CarePlans + \lfloor ureaNitrogen \rfloor \rightarrow Deceased$
15	$activeCarePlans > \lfloor \log(triglycerides) \rfloor \rightarrow Deceased$
16	$health care Expenses < lifetime Condition Length^2 + encounters Lifetime Total Cost \rightarrow Deceased$
17	overlappingMalignantNeo ightarrow Deceased
18	$latitude > ureaNitrogen \lceil albuminMassVolumeInSerumOrPlasma \rceil \rightarrow Deceased$
19	$active Condition Length > erythrocytes Volume In Blood \times \lceil hemoglobin Mass Volume In Blood \rceil \rightarrow Deceased$
20	$\underline{\hspace{1cm}} chronicObstructiveBronc \rightarrow Deceased$
21	$longitude > \sqrt{healthcareCoverage} - encountersCount \rightarrow Deceased$
22	$age > 10^{medicationsActive} - longitude \rightarrow Deceased$
23	$chloride < \lfloor meanChloride \rfloor - lifetimeCarePlans \rightarrow Deceased$
24	$medications Active > \max\{respiratoryRate, \log(latitude)\} \rightarrow Deceased$
25	localizedPrimaryOsteoa ightarrow Deceased
26	rheumatoidArthritis ightarrow Deceased
27	$chronicPain \ \& \ smokesTobaccoDaily ightarrow Deceased$
28	$latitude < \lfloor erythrocyteDistributionWidth \rfloor - meanPainSeverity \rightarrow Deceased$
29	$active Care Plans > 10^{medications Active} / imaging Studies Lifetime \rightarrow Deceased$
30	tubalPregnancy ightarrow Deceased
31	$active Conditions < medications Active^2 - medications Lifetime \rightarrow Deceased$
32	$alcoholism \ \& \ major Depression Disorder ightarrow Deceased$
33	$creatinine < \lceil meanCreatinine \rceil / lifetimeCarePlans \rightarrow Deceased$
34	$health care Coverage < encoutners Lifetime Payer Coverage \times \log(latitude)/\log(10) \rightarrow Deceased$
35	$encountersCount < \min\{DALY, 10^{immunizationsLifetime}\} \rightarrow Deceased$
36	$lifetimeCarePlanLength > age + e^{medicationsLifetime} \rightarrow Deceased$
37	$health care Coverage < active Condion Length^2 - encounters Lifetime Total Cost \rightarrow Deceased$
38	$age > 1/2 \times healthcareExpenses/immunizationsLifetimeCost \rightarrow Deceased$
39	$active Care Plan Length > active Condition Length \times e^{DALY} \rightarrow Deceased$
40	$medications Lifetime < \sqrt{encounters Lifetime Payer Coverage} - age \rightarrow Deceased$

Table 11 Evaluation of Conjectures for Deceased Status Among Those with COVID

on Conjectu	les foi Dece	iseu Status	Aillong
Conjecture	Precision	Support	Lift
1	30.91%	372	4.15
2	24.44%	2954	3.29
3	23.22%	1722	3.12
4	22.47%	632	3.02
5	22.39%	844	3.01
6	21.74%	1490	2.92
7	21.44%	4427	2.88
8	21.24%	2199	2.85
9	21.01%	257	2.82
10	20.90%	799	2.81
11	20.03%	1058	2.69
12	18.25%	548	2.45
13	17.56%	467	2.36
14	17.54%	1898	2.36
15	17.31%	3328	2.33
16	17.23%	940	2.32
17	16.92%	130	2.27
18	16.13%	1091	2.17
19	15.68%	797	2.11
20	14.11%	900	1.90
21	14.08%	781	1.89
22	14.08%	2230	1.89
23	11.99%	884	1.61
24	11.84%	1884	1.59
25	11.76%	2159	1.58
26	11.44%	201	1.54
27	10.54%	607	1.42
28	10.27%	1724	1.38
29	9.39%	213	1.26
30	8.85%	2147	1.19
31	8.22%	4150	1.10
32	7.79%	1129	1.05
33	7.77%	2408	1.04
34	7.73%	634	1.04
35	5.20%	3209	0.70
36	3.89%	4602	0.52
37	3.85%	467	0.52
38	2.65%	339	0.36
39	2.29%	3188	0.31
40	1.30%	1001	0.17
	·	•	

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