

Random vs. Best-First: Impact of Sampling Strategies on Decision Making in Model-Based Diagnosis

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Abstract

Statistical samples, in order to be representative, have to be drawn from a population in a random and unbiased way. Nevertheless, it is common practice in the field of model-based diagnosis to make estimations from (biased) best-first samples. One example is the computation of a few most probable fault explanations for a defective system and the use of these to assess which aspect of the system, if measured, would bring the highest information gain. In this work, we scrutinize whether these statistically not well-founded conventions, that both diagnosis researchers and practitioners have adhered to for decades, are indeed reasonable. To this end, we empirically analyze various sampling methods that generate fault explanations. We study the representativeness of the produced samples wrt. their estimations about fault explanations and how well they guide diagnostic decisions, and we investigate the impact of sample size, the optimal trade-off between sampling efficiency and effectivity, and how approximate sampling techniques compare to exact ones.

1 Introduction

Suppose we intend to predict the outcome of an election and conduct a poll where we ask only, say, university professors for whom they are going to vote. By this strategy, we will most likely not gain insight into the real sentiment in the population wrt. the election. The problem is that professors are most probably not representative of all people. In model-based diagnosis, however, such kind of samples are often used as a basis for making decisions that rule the efficiency of the diagnostic process.

Model-based diagnosis (Reiter 1987) deals with the detection, localization and repair of faults in observed systems such as programs, circuits, knowledge bases or physical devices. One important prerequisite to achieve these goals is the generation of *diagnoses*, i.e., explanations for the faulty system behavior in terms of potentially faulty system components. A sample of diagnoses can be (i) *directly analyzed*, e.g., to manually discover or make estimations about the actual fault (Rodler et al. 2019; Stern et al. 2013), to aid proper algorithm choice (Slaney 2014), or to support users in test case specifications or repair actions (Kalyanpur 2006; Schekotihin, Rodler, and Schmid 2018; Meilicke 2011), or

(ii) *used as an input or guidance to diagnostic algorithms*. We focus on (ii) in this work.

An important class of diagnostic algorithms that are guided by a set of precomputed diagnoses are *sequential diagnosis* (SD) approaches (De Kleer and Williams 1987; De Kleer and Raiman 1993). They use a sample of diagnoses to compute informative system measurements that allow to efficiently and systematically rule out spurious diagnoses until a single or highly probable one remains. Since achieving (global) optimality of the sequence of measurements is intractable in general (Pattipati and Alexandridis 1990), state-of-the-art SD methods usually rely on local optimization (De Kleer, Raiman, and Shirley 1992) using one out of numerous *heuristics* (De Kleer and Williams 1987; Moret 1982; Shchekotykhin et al. 2012; Rodler 2018) as optimality criteria. These heuristics can be seen as functions that, based on a given sample of diagnoses, map measurement candidates to one numeric score each, and finally select the one measurement with the best score. In most cases, these functions use two features of the sample: (F1) the *diagnoses' probabilities*, and (F2) the *diagnoses' predictions of the measurement outcome* (to estimate the probabilities and diagnosis elimination rates of the measurement outcomes).

Literature offers a range of techniques to generate samples of diagnoses, among them ones that return a *specific sample* (Reiter 1987; De Kleer and Williams 1987; Rodler 2020) (which includes exactly a predefined subset of all diagnoses) and others that compute an *unspecific sample*, e.g., in a heuristic (Abreu and Van Gemund 2009), stochastic (Feldman, Provan, and Van Gemund 2008) or simply undefined way (Shchekotykhin et al. 2014) (where no guarantee can be given wrt. diagnosis selection for the sample).

Many existing SD approaches draw on samples of the specific type in that they build upon *best-first* samples, such as maximum-probability or minimum-cardinality diagnoses (Rodler 2015; Shchekotykhin et al. 2012; Gonzalez-Sanchez et al. 2011; De Kleer 1991; De Kleer and Williams 1989; De Kleer and Raiman 1995; Zamir, Stern, and Kalech 2014). While perhaps often being motivated by the desideratum to know the most preferred or likely candidate(s) at any stage of the diagnostic process, e.g., to allow for well-founded stopping criteria, the use of such non-random samples is highly questionable from the statistical viewpoint.

In this work we challenge the validity of the following

statistical law in the domain of model-based diagnosis:

A randomly chosen unbiased sample from a population allows (on average) better conclusions and estimations about the whole population than any other sample.

The particular contributions are: We

- analyze real-world diagnosis cases and gain insight into the quality of *three specific* (best-first, random and, as a baseline, worst-first) and *three unspecific* (approximate best-first / random / worst-first) *sample types*.
- assess a sample type’s quality based on (i) its *theoretical representativeness*, i.e., how well it allows to estimate aspects (F1) and (F2) that determine the heuristic score of measurements, and (ii) its *practical representativeness*, i.e., its performance achieved in a diagnosis session wrt. time and number of measurements.
- investigate the *impact of the (i) sample size, (ii) particular used heuristic, and (iii) tackled diagnosis problem* on the sample’s representativeness.

2 Basics and Problem Motivation

We outline the basics of model-based diagnosis, based on the framework of (Rodler 2015) which is more general (Rodler and Schekotihin 2018) than Reiter’s theory (Reiter 1987).¹

Diagnosis Problem. Assume a diagnosed system, consisting of a set of components $\{c_1, \dots, c_k\}$ and described by a finite set of logical sentences $K \cup B$, where K (possibly faulty sentences) includes knowledge about the behavior of the system components, and B (correct background knowledge) comprises any additional available system knowledge and system observations. More precisely, there is a one-to-one relationship between sentences $s_i \in K$ and components c_i , where s_i describes (only) the nominal behavior of c_i (*weak fault model* (Feldman, Provan, and Van Gemund 2009)). E.g., if c_i is an AND-gate in a circuit, then $s_i := out(c_i) = and(in1(c_i), in2(c_i))$; B in this case might contain sentences stating, e.g., which components are connected by wires, or observed circuit outputs. The inclusion of a sentence s_i in K corresponds to the (implicit) assumption that c_i is healthy. Evidence about the system behavior is captured by sets of positive (P) and negative (N) measurements (Reiter 1987; De Kleer and Williams 1987; Felfernig et al. 2004). Each measurement is a logical sentence; positive ones $p \in P$ must be true and negative ones $n \in N$ must not be true. The former can be, depending on the context, e.g., observations about the system, probes or required system properties. The latter model properties that must not hold for the system, e.g., if K is a biological knowledge base to be debugged, a negative test case might be “every bird can fly” (think of penguins). We call $\langle K, B, P, N \rangle$ a *diagnosis problem instance (DPI)*.

Example 1 (DPI) Assume a DPI stated in propositional logic with $K := \{s_1 : A \rightarrow \neg B, s_2 : A \rightarrow B, s_3 : A \rightarrow \neg C, s_4 : B \rightarrow C, s_5 : A \rightarrow B \vee C\}$. The “system” (here the knowledge base K itself) comprises five

“components” c_1, \dots, c_5 , and the “normal behavior” of c_i is given by the respective sentence $s_i \in K$. No background knowledge ($B = \emptyset$) or positive measurements ($P = \emptyset$) are given from the start. But, there is one negative measurement ($N = \{\neg A\}$), which stipulates that $\neg A$ must *not* be an entailment of the correct system. Note, however, that K (i.e., the assumption that all “components” are normal) in this case does entail $\neg A$ (e.g., due to the sentences s_1, s_2) and thus some sentence (“component”) in K must be faulty. \square

Diagnoses. If the system description along with the positive measurements (under the assumption K that all components are healthy) is inconsistent, i.e., $K \cup B \cup P \models \perp$, or some negative measurement is entailed, i.e., $K \cup B \cup P \models n$ for some $n \in N$, some healthiness assumption(s) of components, i.e., some sentences in K , must be retracted. We call such a set of sentences $D \subseteq K$ a *diagnosis* for the DPI $\langle K, B, P, N \rangle$ iff $(K \setminus D) \cup B \cup P \not\models x$ for all $x \in N \cup \{\perp\}$. We say that D is a *minimal diagnosis* for dpi iff there is no diagnosis $D' \subset D$ for dpi . The set of minimal diagnoses is representative of all diagnoses under the weak fault model (De Kleer, Mackworth, and Reiter 1992), i.e., the set of all diagnoses is equal to the set of all supersets of minimal diagnoses. Thus, diagnosis approaches usually restrict their focus to only minimal diagnoses. We call a diagnosis D^* the *actual diagnosis* iff all elements of D^* are in fact faulty and all elements of $K \setminus D^*$ are in fact correct.

Example 2 (Diagnoses) For our DPI from Ex. 1 we have four minimal diagnoses, given by $D_1 := [s_1, s_3]$, $D_2 := [s_1, s_4]$, $D_3 := [s_2, s_3]$, $D_4 := [s_2, s_5]$. E.g., D_1 is a minimal diagnosis as $(K \setminus D_1) \cup B \cup P = \{s_2, s_4, s_5\}$ is consistent and does not entail the negative measurement $\neg A$. \square

Diagnosis Probabilities. If useful meta information is available that allows to assess the likeliness of failure for system components, the probability of diagnoses (of being the actual diagnosis) can be derived. Specifically, given a function p that maps each sentence (system component) $s \in K$ to its failure probability $p(s) \in (0, 1)$, the probability $p(D)$ of a diagnosis $D \subseteq K$ (under the common assumption of independent component failure) is computed as $p(D) := \prod_{s \in D} p(s) \prod_{s \in K \setminus D} (1 - p(s))$. Each time a new measurement is added to the DPI, probabilities of diagnoses are updated using Bayes’ Theorem (De Kleer and Williams 1987).

Example 3 (Diagnosis Probabilities) Recall the DPI from Ex. 1 and let $\langle p(s_1), \dots, p(s_5) \rangle = \langle .1, .05, .1, .05, .15 \rangle$. Then, the probabilities of all diagnoses from Ex. 2 are $\langle p(D_1), \dots, p(D_4) \rangle = \langle .0077, .0036, .0036, .0058 \rangle$. E.g., $p(D_1)$ is calculated as $.1 * (1 - .05) * .1 * (1 - .05) * (1 - .15)$. The normalized diagnosis probabilities would then be $\langle .37, .175, .175, .28 \rangle$. Note, this normalization makes sense if only a proper subset of all diagnoses is known. \square

Measurement Points. We call a logical sentence a *measurement point (MP)* if it states one (true or false) aspect of the system under consideration. E.g., if the system is a digital circuit, the statement $out(c_i) = 1$, which states that the output of gate c_i is high, is an MP. In case of the system being, say, a knowledge base, $\forall X (bird(X) \rightarrow canFly(X))$ is an MP. Assuming an oracle orcl (e.g., an engineer for a circuit, or a domain expert for a knowledge base) that is knowledge-

¹This framework allows to represent things that must *not* be true for a diagnosed system, which is helpful, e.g., for diagnosing knowledge bases or ontologies (Shchekotykhin et al. 2012).

able about the system, one can send to orcl MPs m and orcl will classify each m as either a positive or a negative measurement, i.e., $m \mapsto \text{orcl}(m)$ where $\text{orcl}(m) \in \{P, N\}$.

Measurements to Discriminate between Diagnoses. MPs are useful for identifying the actual diagnosis among multiple diagnoses for a DPI. Hence, given a set of diagnoses \mathbf{D} for a DPI to discriminate between, the MPs m of particular interest are those for which each classification $\text{orcl}(m)$ is inconsistent with some diagnosis in \mathbf{D} (De Kleer and Williams 1987; Rodler 2015). We call such MPs *informative* (wrt. \mathbf{D}). In other words, each outcome of a measurement for some informative MP will invalidate some diagnosis.

Each MP m partitions any set of (minimal) diagnoses \mathbf{D} into subsets \mathbf{D}_m^+ , \mathbf{D}_m^- and \mathbf{D}_m^0 : (i) Each $D \in \mathbf{D}_m^+$ is consistent (only) with $\text{orcl}(m) = P$ (*diagnoses predicting positive outcome*), (ii) each $D \in \mathbf{D}_m^-$ is consistent (only) with $\text{orcl}(m) = N$ (*diagnoses predicting negative outcome*), and (iii) each $D \in \mathbf{D}_m^0$ is consistent with both outcomes $\text{orcl}(m) \in \{P, N\}$ (*uncommitted diagnoses*). Thus, an MP m is informative iff both \mathbf{D}_m^+ (diagnoses invalidated if $\text{orcl}(m) = N$) and \mathbf{D}_m^- (diagnoses invalidated if $\text{orcl}(m) = P$) are non-empty sets.

(Estimated) Properties of Measurement Points. Since not all informative MPs are equally utile, the consideration of additional properties of MPs enables a more fine-grained preference rating of MPs. In fact, if \mathbf{D} includes all diagnoses for the given DPI, the partition $\langle \mathbf{D}_m^+, \mathbf{D}_m^-, \mathbf{D}_m^0 \rangle$ allows to determine, for each measurement outcome $c \in \{P, N\}$, its *diagnosis elimination rate* $er(\text{orcl}(m) = c)$ as well as its *probability* $p(\text{orcl}(m) = c)$ (Rodler 2018):

$$\begin{aligned} er_m^+ &:= er(\text{orcl}(m) = P) = \frac{|\mathbf{D}_m^-|}{|\mathbf{D}|} \\ er_m^- &:= er(\text{orcl}(m) = N) = \frac{|\mathbf{D}_m^+|}{|\mathbf{D}|} \\ p_m^+ &:= p(\text{orcl}(m) = P) = P_m^+ + \frac{1}{2}P_m^0 \\ p_m^- &:= p(\text{orcl}(m) = N) = P_m^- + \frac{1}{2}P_m^0 \end{aligned}$$

where $P_m^X := \sum_{D \in \mathbf{D}_m^X} p(D)$ for $X \in \{+, -, 0\}$.

In practice, the calculation of all diagnoses is often infeasible and diagnosis systems rely on a subset of the minimal diagnoses \mathbf{D} to *estimate* these properties of MPs. In the following, we denote by $\hat{er}_{m,\mathbf{D}}^+$ and $\hat{er}_{m,\mathbf{D}}^-$ the *estimated elimination rate* for positive and negative measurement outcome for MP m computed based on \mathbf{D} . Similarly, we refer by $\hat{p}_{m,\mathbf{D}}^+$ and $\hat{p}_{m,\mathbf{D}}^-$ to the *estimated probability* of a positive and negative measurement outcome for m and \mathbf{D} . Importantly, these estimated values depend on *both* the MP m and the used sample \mathbf{D} of diagnoses. Note that all four estimates attain values in $[0, 1]$ for any MP m , and in $(0, 1)$ if the MP m is informative. Moreover, $\hat{p}_{m,\mathbf{D}}^+ + \hat{p}_{m,\mathbf{D}}^- = 1$ and $\hat{er}_{m,\mathbf{D}}^+ + \hat{er}_{m,\mathbf{D}}^- \leq 1$ where the difference $1 - (\hat{er}_{m,\mathbf{D}}^+ + \hat{er}_{m,\mathbf{D}}^-)$ is the rate of uncommitted diagnoses, which are not affected by the measurement at m .

Example 4 (Measurement Points & Properties) Assume our DPI from Ex. 1 and let all minimal diagnoses be known, i.e., $\mathbf{D} = \{D_1, \dots, D_4\}$ (cf. Ex. 2). Then, e.g., $m_1 := A \rightarrow C$ is an informative MP wrt. \mathbf{D} since $\mathbf{D}_{m_1}^+ = \{D_1, D_3\} \neq \emptyset$ and $\mathbf{D}_{m_1}^- = \{D_2, D_4\} \neq \emptyset$. E.g., $D_1 \in \mathbf{D}_{m_1}^+$ because $(K \setminus D_1) \cup$

$B \cup P = \{s_2, s_4, s_5\} \supset \{A \rightarrow B, B \rightarrow C\} \models m_1$ and thus m_1 can be no negative measurement under the assumption D_1 . Similarly, $D_2 \in \mathbf{D}_{m_1}^-$ due to $(K \setminus D_2) \cup B \cup (P \cup \{m_1\}) = \{s_2, s_3, s_5, m_1\} \supset \{A \rightarrow \neg C, A \rightarrow C\} \models \neg A$ where $\neg A$ is a negative measurement; hence, m_1 can be no positive measurement under the assumption D_2 . In contrast, e.g., $m_2 := B$ is a non-informative MP because $\mathbf{D}_{m_2}^+ = \emptyset$.

Assuming the (normalized) probabilities from Ex. 3, we obtain probabilities $\hat{p}_{m_1,\mathbf{D}}^+ = .545$, $\hat{p}_{m_1,\mathbf{D}}^- = .455$ and elimination rates $\hat{er}_{m_1,\mathbf{D}}^+ = .5$, $\hat{er}_{m_1,\mathbf{D}}^- = .5$ for m_1 . Note: (1) If we have at hand a different sample \mathbf{D} , the estimations for one and the same MP might vary substantially. E.g., suppose $\mathbf{D} = \{D_1, D_2, D_3\}$; then $\hat{p}_{m_1,\mathbf{D}}^+ = .758$, $\hat{p}_{m_1,\mathbf{D}}^- = .242$ and $\hat{er}_{m_1,\mathbf{D}}^+ \approx 0.33$, $\hat{er}_{m_1,\mathbf{D}}^- \approx .67$. (2) Smaller (larger) samples will tend to provide a sparser (richer) selection of MP candidates. E.g., m_1 becomes non-informative if $\mathbf{D} = \{D_1, D_3\}$, and thus might be disregarded by diagnosis systems. \square

Evaluating Measurement Points by Heuristics. To quantitatively assess the preferability of different MPs, state-of-the-art diagnosis systems rely on heuristics that perform a one-step-lookahead analysis of MPs (De Kleer, Raiman, and Shirley 1992). A *heuristic* h is a function that maps each MP m to a real-valued score $h(m)$ (Rodler 2016), where $h(m)$ quantifies the *utility of the expected situation after knowing the outcome for MP m* . The MP with the best score as per the used heuristic is then chosen as a next query to the oracle.

Well-known heuristics incorporate exactly the two discussed features, i.e., the estimated elimination rates and estimated probabilities, into their computations (Rodler 2018). So, different heuristics correspond to different functions of these estimates, e.g.: (1) *information gain (ENT)* (De Kleer and Williams 1987) uses solely the probabilities and prefers MPs where $P_m^0 = 0$ and $|\hat{p}_{m,\mathbf{D}}^+ - \hat{p}_{m,\mathbf{D}}^-|$ is minimal; (2) *split-in-half (SPL)* (Shchekotykhin et al. 2012) considers only the elimination rates and favors MPs with $\hat{er}_{m,\mathbf{D}}^+ + \hat{er}_{m,\mathbf{D}}^- = 1$ and minimal $|\hat{er}_{m,\mathbf{D}}^+ - \hat{er}_{m,\mathbf{D}}^-|$ (Rodler 2016); (3) *risk optimization (RIO)* (Rodler et al. 2013) takes into account both features by computing a dynamically re-weighted function of ENT and SPL; (4) *most probable singleton (MPS)* (Rodler 2018, 2016) also regards both features by giving preference to MPs that maximize the probability of a maximal elimination rate. For details on heuristics see (Rodler 2018, 2016) for theoretical analyses and (Shchekotykhin et al. 2012; Rodler and Schmid 2018; Rodler et al. 2013; Rodler and Eichholzer 2019) for empirical evaluations.

Example 5 (Heuristics) Reconsider our DPI from Ex. 1 and the MP m_1 from Ex. 4, and let $\mathbf{D} = \{D_1, \dots, D_4\}$. Further, let $m_3 := A \wedge \neg B \rightarrow C$. Note, m_3 is informative (wrt. \mathbf{D}), $\mathbf{D}_{m_3}^+ = \{D_1, D_2, D_3\}$, $\mathbf{D}_{m_3}^- = \{D_4\}$, and the estimations $\hat{p}_{m_3,\mathbf{D}}^+ = .72$, $\hat{p}_{m_3,\mathbf{D}}^- = .28$ and $\hat{er}_{m_3,\mathbf{D}}^+ = .25$, $\hat{er}_{m_3,\mathbf{D}}^- = .75$. Hence, given the two MP candidates $\{m_1, m_3\}$, the heuristic SPL would select m_1 (since a half of the known diagnoses are eliminated for each outcome). Similarly, ENT would prefer m_1 to m_3 (because for m_1 roughly a half of the probability mass is eliminated for each outcome).

However, assume a used sampling technique outputs the sample $\mathbf{D} = \{D_2, D_3, D_4\}$. In this case, we obtain the prob-

ability estimates $\hat{p}_{m1,D}^+ = .28, \hat{p}_{m1,D}^- = .72$ as well as $\hat{p}_{m3,D}^+ = .55, \hat{p}_{m3,D}^- = .45$. So, using ENT, the chosen MP would be m_3 (the worse MP, as shown above). If sampling would yield $\mathbf{D} = \{D_2, D_4\}$, then m_1 would not even be an informative MP (wrt. \mathbf{D}) on the one hand, and m_3 would be the (theoretically) optimal MP as per SPL on the other hand. This example shows the dramatic impact the used sampling technique can have on diagnostic decisions. \square

Sequential Diagnosis (SD) aims at generating a sequence of informative MPs such that a single (highly probable) diagnosis remains for the given DPI, while minimizing the number of MPs needed (oracle inquiries are usually expensive). A generic SD process iterates through the following steps until (the Bayes-updated) $p(D)$ for some $D \in \mathbf{D}$ exceeds a probability threshold σ : (S1) Generate a sample of minimal diagnoses \mathbf{D} for the current DPI. (S2) Choose a (heuristically optimal) informative MP m wrt. \mathbf{D} (using a selection heuristic h). (S3) Ask the oracle orcl to classify m . (S4) Use the classification $\text{orcl}(m)$ to update the DPI, by adding m to the positive measurements if $\text{orcl}(m) = P$ and to the negative measurements if $\text{orcl}(m) = N$.

3 Evaluation

We conducted extensive experiments on a dataset of real-world diagnosis cases (Sec. 3.1) to study six different diagnosis sample types (Secs. 3.2 and 3.3) wrt. the accuracy of estimations and diagnostic efficiency (Sec. 3.4). The experiments (Sec. 3.6) target five specific research questions (Sec. 3.5) and their results are analyzed in detail (Sec. 3.7).

3.1 Dataset

In our experiments we drew upon the set of real-world diagnosis problems from the domain of knowledge-base debugging shown in Tab. 1. Note, every model-based diagnosis problem (according to Reiter’s theory (Reiter 1987)) can be represented as a knowledge-base debugging problem (Rodler and Schekotihin 2018), which is why considering knowledge-base debugging problems is without loss of generality. To obtain a representative dataset we chose it in a way it covers a variety of different problem sizes, theorem proving complexities, and diagnostic metrics (number and size of diagnoses, number of components). These metrics are depicted in the columns of Tab. 1. In order to implement the random sampling of diagnoses, another requirement to the dataset was that all the used problems allow the computation of *all* minimal diagnoses within tolerable time for our experiments (single digit number of minutes).

3.2 Sample Types

We examined the following types of diagnosis samples: (T1) best-first (*bf*), (T2) random (*rd*), (T3) worst-first (*wf*), (T4) approximate best-first (*abf*), (T5) approximate random (*ard*), and (T6) approximate worst-first (*awf*). By “best-first” / “worst-first”, we mean the most / least probable minimal diagnoses. Types T3 and T6 serve as baselines. We refer to T1, T2 and T3 as *specific sample types* because we know the properties of the sample (exactly the k best or worst diagnoses, or k unbiased random ones) in advance by employing

Table 1: Dataset used in experiments (sorted by 2nd column).

KB K	$ K $	expressivity ¹⁾	#D/min/max ²⁾
University (U) ³⁾	50	$SOIN^{(D)}$	90/3/4
IT ⁴⁾	140	$SROIQ$	1045/3/7
UNI ⁴⁾	142	$SROIQ$	1296/5/6
MiniTambis (M) ³⁾	173	$ALCN$	48/3/3
Transportation (T) ³⁾	1300	$ALCH^{(D)}$	1782/6/9
Economy (E) ³⁾	1781	$ALCH^{(D)}$	864/4/8
DBpedia (D) ⁵⁾	7228	$ALCH\mathcal{F}^{(D)}$	7/1/1
Cton (C) ⁶⁾	33203	\mathcal{SHF}	15/1/5

1): Logical expressivity (Baader et al. 2007); the higher it is, the higher is the complexity of consistency checking (diagnosis computation) for this logic.

2): #D/min/max denotes the number/the minimal size/the maximal size of minimal diagnoses for the DPI resulting from KB K .

3): Hardest diagnosis problems from evaluations in (Shchekotykhin et al. 2012), which were also used, e.g., in (Horridge, Parsia, and Sattler 2009; Ji et al. 2014).

4): Diagnosis problems studied in (Rodler et al. 2019; Rodler 2020).

5): Faulty version of DBpedia ontology, see <https://bit.ly/2ZO2qYZ>.

6): Diagnosis problem used in scalability tests in (Shchekotykhin et al. 2012).

(expensive) sampling techniques that guarantee these properties. On the other hand, we call *T4, T5 and T6 unspecific sample types* and adopt (usually less costly) heuristic techniques to provide them. Throughout, we denote a sample of type Ti including k minimal diagnoses by $S_{Ti,k}$.

3.3 Sampling Techniques

The methods we used to generate the samples for a given DPI $dpi = \langle K, B, P, N \rangle$ are:

T1: We used uniform-cost HS-Tree (Rodler 2015, Sec. 4.6) and stopped it after k diagnoses were computed. Due to the best-first property of the algorithm, these are provenly (Rodler 2015, Prop. 4.17) the k diagnoses with the highest probability among all minimal diagnoses.

T2, T3: We generated all² minimal diagnoses **allD** for dpi (this can be done by any sound and complete diagnosis computation method, e.g., HS-Tree (Reiter 1987)). For T2, we selected k random elements from this set by means of the Java (v1.8) pseudorandom number generator. For T3, we picked the k diagnoses with lowest probability.

T4, T5, T6: We used Inv-HS-Tree (Shchekotykhin et al. 2014) to supply the samples. First, we added all $s \in K$ to a list L . For T5, we randomly shuffled L . For T4 and T6, we sorted L in descending and ascending order of probability $p(s)$, respectively. Finally, we let plain Inv-HS-Tree operate on this list L to supply a sample of size k .

3.4 Evaluating Samples

We evaluate sample types based on what we call their theoretical and practical representativeness:

Theoretical Representativeness (T-Rep): A sample type Ti is the more representative, the better the (i) probability estimates $\langle \hat{p}_{m,D}^+, \hat{p}_{m,D}^- \rangle$ for MPs m match the respec-

²This is generally intractable (Bylander et al. 1991). So, this approach to random sampling is not viable in practice and just used for evaluation purposes. As said in Sec. 3.1, we chose our dataset so that computation of **allD** was feasible.

tive actual values $\langle p_m^+, p_m^- \rangle$, (ii) elimination rate estimates $\langle \hat{er}_{m,D}^+, \hat{er}_{m,D}^- \rangle$ for MPs m match the respective actual values $\langle er_m^+, er_m^- \rangle$ for samples $D = S_{Ti,k}$.

Practical Representativeness (P-Rep): A sampling technique Ti is the more representative, the lower the (i) number of measurements required, (ii) time needed for sampling (diagnosis computation) in a sequential diagnosis session until the actual diagnosis is isolated from spurious ones, where $D = S_{Ti,k}$ in each sequential diagnosis iteration.

3.5 Research Questions

We investigate the following research questions:

- R1 Which type of sample is best in terms of T-Rep?
- R2 Which type of sample is best in terms of P-Rep?
- R3 Are the results wrt. R1 and R2 consistent over different
 - (a) sample sizes, (b) measurement selection heuristics, and (c) diagnosis problem instances?
- R4 Does larger sample size imply better representativeness?
- R5 Does better T-Rep translate to better P-Rep?

3.6 Experiments

We ran two experiments, EXP1 and EXP2, to study our research questions. Common to both of them are the following settings: (i) We defined one DPI $dpi_K := \langle K, \emptyset, \emptyset, \emptyset \rangle$ for each K in Tab. 1. That is, we assumed each sentence (component) in K to be possibly faulty and left the background knowledge and the measurements void to begin with. To each $s \in K$, we randomly assigned a fault probability $p(s) \in (0, 1)$ in a way that syntactically equally (more) complex sentences have an equal (higher) probability (cf. (Shchekotykhin et al. 2012)). E.g., in our DPI from Ex. 1, elements of $\{s_1, s_3\}$ (one implication, one negation) and $\{s_2, s_4\}$ (one implication), respectively, would each be allocated the same probability, and the former two would have a higher probability than the latter (cf. Ex. 3). (ii) We pre-computed all minimal diagnoses **allD** for each DPI dpi_K . (iii) We used all sample types Ti for $i \in \{1, \dots, 6\}$ (cf. Sec. 3.2). (iv) We used sample sizes (numbers of generated minimal diagnoses) $k \in \{2, 6, 10, 20, 50\}$.

The specific settings for each experiment were:

EXP1: (T-Rep) For each dpi_K , for each k , and for each Ti , we computed a sample $D = S_{Ti,k}$. We used (i) **D** to compute probability and elimination rate estimates $\langle \hat{p}_{m,D}^+, \hat{p}_{m,D}^- \rangle$ and $\langle \hat{er}_{m,D}^+, \hat{er}_{m,D}^- \rangle$, and (ii) **allD** to compute $\langle p_m^+, p_m^- \rangle$ and $\langle er_m^+, er_m^- \rangle$ for 50 (if so many, otherwise for all) randomly selected informative MPs wrt. **D**. For each such MP, we thus had four estimates and four corresponding actual values, that we could compare against one another.

EXP2: (P-Rep) For each dpi_K , for each k , for each Ti , and for each of the four heuristics $h \in \{\text{ENT, SPL, RIO, MPS}\}$ (cf. Sec. 2), we executed 10 diagnosis sessions (loop $S1-S4$, Sec. 2) while in each session (i) searching for a different randomly selected target diagnosis $D^* \in \text{allD}$ for dpi_K , (ii) starting from the initial problem dpi_K , (iii) with stop criterion $\sigma = 1$ (loop until a single minimal diagnosis remains, i.e., all others have been ruled out). At this, in each loop iteration, at step $S1$, a sample $D = S_{Ti,k}$ is drawn for the current DPI, at step $S2$, an optimal informative MP wrt.

h is selected, and at step $S3$, an automated oracle classifies each MP in a way the target diagnosis D^* is not ruled out. For our analyses, we recorded (sampling) times and number of measurements (i.e., loop iterations) throughout a session.

3.7 Results

From our experiments, we obtained two large datasets, with $6 * 8 * 5 = 240$ (EXP1) and $6 * 8 * 5 * 4 = 960$ (EXP2) factor combinations for the factors sample type (6 levels), diagnosis problem (8), sample size (5), and heuristic (4).³

Presentation. Tab. 2 shows rankings of the sample types over different subsets of all factor combinations (referred to as *scenarios*; left column of the table). E.g., scenario “all” means all 240 (EXP1) / 960 (EXP2) cases aggregated, whereas “ $k = 20$ ” denotes exactly the $240 : 5 = 48$ (EXP1) / $960 : 5 = 192$ (EXP2) cases where the sample size was set to 20. Results from EXP1 are depicted in the top part of the table (first ten rows); results from EXP2 in the bottom part. A sample type Ti being ranked prior to type Tj (middle table column) means that Ti was better than Tj in more factor combinations of the respective scenario than vice versa. Equally ranked sample types are written in parentheses. The meaning of “better” (*criterion* for comparison; rightmost table column) is a higher Pearson correlation coefficient between estimated and real values for elimination rate (E) and, respectively, probability (P) estimations (cf. T-Rep in Sec. 3.4), and a lower avg. number of measurements (M) and, respectively, a lower avg. sample computation time (T) in diagnosis sessions (cf. P-Rep in Sec. 3.4).⁴ The idea behind this representation is to give the user of a diagnosis system guidance how to set parameters (diagnosis computation algorithm, number of computed diagnoses, measurement selection heuristic) in order to have the highest chance of achieving best estimations (EXP1) / efficiency (EXP2).

Tab. 3 lists the best (ranked) sample types wrt. overall time per diagnosis session in EXP2 (cumulated system computation time plus cumulated time for all measurements) for different scenarios and assumptions (1min, 10min) of measurement conduction times. The two rightmost columns (“adj”) show hypothetical results under the assumption that sample types $T2$ (*rd*) and $T3$ (*wf*)—which we naively simulated by means of brute force diagnosis computation in our experiments (cf. Sec. 3.3)—were as efficiently computable as sample type $T1$ (*bf*). This allows to assess the added value of, e.g., *efficient* random diagnosis sampling techniques.

Discussion. We address each research question in turn:

R1:⁵ (*Elimination rate, criterion E, Tab. 2*) We see that *rd* is

³Please see code appendix for information on code, computing infrastructure, and raw data.

⁴Tab. 2 does *not* inform about *how much better (worse)* one Ti was than another, but only that it was a preferred choice to the other *in more (less) cases* (of a scenario). And, a higher ranked strategy is not necessarily *always* better than a lower ranked one.

⁵Remarks wrt. R1: (1) We had to leave out the $k = 2$ scenarios as there were too few informative MPs which made these scenarios not reliably analyzable. (2) Values and rankings for other types of correlation coefficients (i.e., Spearman and Kendall) were very similar to the presented (Pearson) results. (3) Most correlation coefficients were statistically significant ($\alpha = 0.05$), except for a few

Table 2: T-Rep and P-Rep: Rankings of sample types for various scenarios (EXP1 & EXP2).

scenario	(best)	ranking					(worst)	criterion
all	<i>rd</i>	<i>wf</i>	<i>bf</i>	<i>awf</i>	(<i>abf</i>	<i>ard</i>)		E
$k = 6$	<i>bf</i>	<i>wf</i>	(<i>rd</i>	<i>awf</i>)	<i>abf</i>	<i>ard</i>		E
$k = 10$	<i>rd</i>	<i>wf</i>	<i>bf</i>	<i>awf</i>	<i>abf</i>	<i>ard</i>		E
$k = 20$	<i>rd</i>	<i>wf</i>	<i>bf</i>	<i>awf</i>	(<i>abf</i>	<i>ard</i>)		E
$k = 50$	<i>rd</i>	<i>wf</i>	<i>awf</i>	<i>bf</i>	<i>ard</i>	<i>abf</i>		E
all	<i>bf</i>	<i>rd</i>	<i>awf</i>	<i>abf</i>	<i>ard</i>	<i>wf</i>		P
$k = 6$	<i>bf</i>	(<i>abf</i>	<i>rd</i>	<i>ard</i>)	<i>awf</i>	<i>wf</i>		P
$k = 10$	<i>bf</i>	<i>rd</i>	(<i>abf</i>	<i>awf</i>)	(<i>ard</i>	<i>wf</i>)		P
$k = 20$	<i>bf</i>	<i>rd</i>	<i>awf</i>	(<i>abf</i>	<i>ard</i>	<i>wf</i>)		P
$k = 50$	<i>bf</i>	<i>rd</i>	<i>awf</i>	<i>ard</i>	<i>wf</i>	<i>abf</i>		P
all	<i>bf</i>	<i>ard</i>	<i>abf</i>	<i>rd</i>	<i>awf</i>	<i>wf</i>		M
$k = 2$	<i>bf</i>	<i>abf</i>	<i>ard</i>	<i>awf</i>	<i>rd</i>	<i>wf</i>		M
$k = 6$	<i>bf</i>	<i>rd</i>	<i>ard</i>	<i>abf</i>	<i>awf</i>	<i>wf</i>		M
$k = 10$	<i>rd</i>	<i>abf</i>	<i>ard</i>	<i>bf</i>	<i>awf</i>	<i>wf</i>		M
$k = 20$	<i>ard</i>	<i>abf</i>	<i>awf</i>	<i>rd</i>	<i>bf</i>	<i>wf</i>		M
$k = 50$	<i>ard</i>	<i>rd</i>	<i>awf</i>	<i>bf</i>	<i>abf</i>	<i>wf</i>		M
$h = \text{ENT}$	<i>bf</i>	<i>abf</i>	<i>ard</i>	<i>awf</i>	<i>rd</i>	<i>wf</i>		M
$h = \text{SPL}$	<i>bf</i>	<i>ard</i>	<i>abf</i>	<i>rd</i>	<i>awf</i>	<i>wf</i>		M
$h = \text{RIO}$	<i>rd</i>	<i>ard</i>	<i>awf</i>	<i>bf</i>	<i>abf</i>	<i>wf</i>		M
$h = \text{MPS}$	<i>ard</i>	<i>abf</i>	<i>rd</i>	<i>awf</i>	<i>wf</i>	<i>bf</i>		M
all	<i>awf</i>	<i>bf</i>	(<i>abf</i>	<i>ard</i>)	<i>rd</i>	<i>wf</i>		T
$k = 2$	<i>abf</i>	(<i>ard</i>	<i>awf</i>)	<i>bf</i>	<i>rd</i>	<i>wf</i>		T
$k = 6$	<i>awf</i>	(<i>abf</i>	<i>ard</i>)	<i>bf</i>	(<i>rd</i>	<i>wf</i>)		T
$k = 10$	<i>awf</i>	<i>abf</i>	(<i>ard</i>	<i>bf</i>)	<i>rd</i>	<i>wf</i>		T
$k = 20$	<i>bf</i>	<i>ard</i>	<i>awf</i>	<i>abf</i>	<i>rd</i>	<i>wf</i>		T
$k = 50$	<i>bf</i>	<i>wf</i>	(<i>awf</i>	<i>rd</i>)	<i>ard</i>	<i>abf</i>		T
$h = \text{ENT}$	<i>awf</i>	<i>abf</i>	<i>bf</i>	<i>ard</i>	<i>rd</i>	<i>wf</i>		T
$h = \text{SPL}$	(<i>abf</i>	<i>awf</i>	<i>bf</i>)	<i>ard</i>	<i>rd</i>	<i>wf</i>		T
$h = \text{RIO}$	<i>awf</i>	(<i>abf</i>	<i>ard</i>)	<i>bf</i>)	<i>rd</i>	<i>wf</i>		T
$h = \text{MPS}$	<i>bf</i>	<i>awf</i>	<i>ard</i>	<i>abf</i>	<i>rd</i>	<i>wf</i>		T

Table 3: Best sample types wrt. overall sequential diagnosis time for various scenarios (EXP2).

	best sample type (given that time for each measurement = t)			
scenario	$t = 1\text{min}$	$t = 10\text{min}$	$t = 1\text{min (adj)}$	$t = 10\text{min (adj)}$
all data	<i>bf</i>	<i>bf</i>	<i>bf</i>	<i>bf</i>
$k = 2$	<i>bf</i>	<i>bf</i>	<i>bf</i>	<i>bf</i>
$k = 6$	<i>bf</i>	<i>bf</i>	<i>bf</i>	<i>bf</i>
$k = 10$	<i>abf</i>	<i>abf</i>	<i>abf</i>	(<i>rd, abf</i>)
$k = 20$	<i>awf</i>	<i>bf</i>	<i>awf</i>	<i>bf</i>
$k = 50$	<i>bf</i>	<i>bf</i>	<i>rd</i>	<i>rd</i>
$h = \text{ENT}$	<i>bf</i>	<i>bf</i>	<i>bf</i>	<i>bf</i>
$h = \text{SPL}$	<i>bf</i>	<i>bf</i>	<i>bf</i>	<i>bf</i>
$h = \text{RIO}$	<i>bf</i>	<i>ard</i>	<i>rd</i>	(<i>ard, bf</i>)
$h = \text{MPS}$	<i>ard</i>	<i>ard</i>	<i>ard</i>	<i>ard</i>

the sample type of choice, as one would expect. In numbers, the median correlation coefficients over all cases per scenario for (best, worst) sample type for $k \in \{6, 10, 20, 50\}$ were $\{(0.76, 0.5), (0.83, 0.52), (0.95, 0.7), (0.98, 0.85)\}$, which reveals that estimations were altogether pretty good

$k = 6$ scenarios and some scattered $k = 10$ cases.

for all sampling techniques. However, for $k \geq 20$, coefficients for *rd* manifested a significantly lower variance than in case of all other techniques, i.e., all coefficients for *rd* concentrated in the interval $[0.9, 1]$, whereas lowest coefficients for all other techniques lay between less than 0.5 and 0.7. Moreover, it stands out that *wf* allowed almost as accurate estimations as *rd*. A likely explanation for these favorable results of *wf* is that there is usually a large number of minimal diagnoses with a very small probability, which is why the “sub-population” from which the *wf* diagnoses are “selected” tends to be larger (and thus more representative) than for other sample types, except for *rd* (where diagnoses are drawn at random from the *full* population). Finally, it is interesting that approximate methods (*awf*, *ard*, *abf*) produced less representative samples than exact ones. And, although *rd* comes out on top for E, its approximate counterpart *ard* shows the worst results. That is, Inv-HS-Tree with a random sorting of its input (cf. Sec. 3.3) does not allow to simulate a random selection of diagnoses.

(Probability, criterion P, Tab. 2) Here, *bf* proved to be the predominantly superior technique in all depicted scenarios, whereas *rd* was, surprisingly, only the second best method. Closer analyses of the data revealed that the explanation for this is that often few of the most probable diagnoses already accounted for a major part of the overall probability mass, which is why they are more reliable for estimations of P than a random sample. For the same reason, *wf* samples turned out to be the least preferable means to estimate P. The medians of the correlation coefficients over all cases per scenario for (best, worst) sample type for $k \in \{6, 10, 20, 50\}$ were $\{(0.93, 0.6), (0.87, 0.64), (0.98, 0.74), (0.99, 0.86)\}$. Thus, again, all sampling methods enabled pretty decent estimations, even for small sample sizes.

R2: (Number of measurements, criterion M, Tab. 2) We find that *bf* was the best strategy if all data is considered; and it was the most suitable choice for heuristics ENT and SPL and for small sample sizes $\{2, 6\}$. On the other hand, it was the worst choice for the MPS heuristic where it led to substantial overheads (of up to $>100\%$) compared to other sample types, especially for large sample sizes. E.g., for the diagnosis problem U and $k = 50$, in a diagnosis session using *bf* 58 measurements had to be conducted to identify the actual fault vs. only 25 measurements if *rd* was used instead. What is somewhat surprising is that *bf* decidedly outperformed *rd* in the SPL scenarios, although the SPL function does not use any probabilities (where *bf* leads to better estimations), but solely the elimination rate (where *rd* produces better estimates). Further analyses are needed to better understand this phenomenon. Overall, *rd* compares favorably only against *awf* and *wf*, but its performance depends largely on the used heuristic. For RIO it is even the sample type of choice, and for MPS it clearly overcomes *bf*. For all four heuristics, one of the approximate methods was the second best method, among which *ard* led to good performance most consistently. In comparison with *rd*, *ard* was only (slightly) outweighed for RIO, but prevails for the other three heuristics. When considering large samples (20 or 50 diagnoses), *ard* even turned out to be the overall winner. This indicates that the QuickXPlain-based approximate

random algorithm, in spite of its rather poor estimations (cf. E and P in Tab. 2), tends to be no less effective than a real random strategy. Also, observe that *wf* was in fact the least favorable option in quasi all scenarios.

(*Time for diagnosis session, criterion T, Tab. 2*) Due to the brute force approach we used in our experiments to generate samples of type *rd* and *wf*, it comes as no surprise that these two methods perform most poorly in terms of T. When drawing our attention to the best strategies, we find that, in all but one ($h = \text{SPL}$) of the shown scenarios, it is a different sample type that exhibited lowest time (T) than the one that manifested the lowest number of measurements (M). Hence, there appears to be a *time-information trade-off* in diagnosis sampling—or: whenever the sampling process is most efficient (on avg.), the measurements arising from the sample are not most effective (on avg.). In particular, we recognize that, if an exact method is best for T (M), then an approximate method is best for M (T).

(*Diagnosis session time, criteria T & M combined, Tab. 3*) As the outcome for *R2* is not clear-cut when viewing M and T separately, we investigate their combined effect, i.e., the overall (avg.) time for diagnosis sessions for the different sample types. In brief, the conclusions are: (i) For small sample size below 10, go with *bf*. (ii) For sample size 10, use *abf*. (iii) For sample size 20, take *awf* if the expected time for conducting measurements is low, and take *bf* else. (iv) Unless there is an efficient method for *rd*, use *bf* for large sample size (50), otherwise use *rd*. (v) For ENT or SPL, adopt *bf*. (vi) For RIO, if measurement time is short, use *bf* if there is no efficient method for *rd*, else use *rd*; if measuring takes longer, use *ard*. (vii) For MPS, use *ard*.

R3: For T-Rep, we observe pretty consistent (ranking) results over all sample sizes (cf. often equal entries in each column for each of the E and P criteria in Tab. 2). There is more variation when comparing results for different diagnosis problems. Nevertheless, results are fairly stable wrt. the winning strategy: *rd* is in all cases the best (75 %) or second best (25 %) sample type for E, and *bf* is in all but one case the best (63 %) or second best (25 %) sample type for P. For P-Rep, we see more of a fluctuation over different sample sizes and heuristics, as discussed for *R2* above (cf. variation over entries of each column for M and T in Tab. 2). Examining results over different diagnosis problems reveals a similar picture, where however the rankings for T are decidedly more stable than those for M, meaning that relative sampling times are less affected by the particular problem instance than the informativeness of the samples.

R4: Our data indicates a clear trend that increasing sample size leads to better T-Rep (cf. discussion of *R1*). However, it also suggests that there is no general significant positive effect of larger sample size on P-Rep. While this is obvious for sampling time (T), i.e., generating more diagnoses cannot take less time, it is less so for the number of measurements (M). In fact, we even measured increases wrt. M in some cases (e.g., for MPS) as a result to drawing larger samples. This is in line with similar findings, albeit for lower sample sizes or other types of diagnosis problems, reported by (Rodler and Schmid 2018; De Kleer and Raiman 1995).

R5: From our data, we cannot generally conclude that a bet-

ter T-Rep implies a better P-Rep (see discussion on *R1*, *R2* and *R3*). E.g., observe the performance of *ard* in the top (criteria E,P) vs. bottom (criteria M,T) part of Tab. 2. The likely cause of this is that all common measurement selection heuristics are based on a one-step-lookahead (De Kleer, Raiman, and Shirley 1992), where the approximate character of this analysis might lower the benefit of good estimations.

4 Research Limitations

Our evaluations do not come without limitations. In brief, there are the following threats to validity:⁶ 1. For feasibility reasons, we (i) could not use *all* diagnoses, but only all minimal ones, to determine the real values (EXP1), and (ii) had to rely on problem instances that allow the generation of all minimal diagnoses in reasonable time. 2. We focused on binary-outcome measurements which are common in some but not all diagnosis sub-domains, e.g., in knowledge base debugging (Schekotihin, Rodler, and Schmid 2018), circuit diagnosis (De Kleer and Williams 1987), or matrix-based methods (Shakeri et al. 2000).^{*} 3. We did not evaluate *bf* sample types including minimum-cardinality diagnoses, but concentrated on most probable ones.^{*} 4. To keep the size of our dataset manageable, we (i) omitted less commonly used existing heuristics, and (ii) included only a subset of all diagnosis computation methods in literature in our analyses.^{*}

5 Conclusions

This work addresses an important and fundamental question for model-based diagnosis, i.e., whether the fully biased diagnosis samples primarily used in the field provide a reasonable basis for decision-making in spite of not being in line with statistical practices. The bottom line of our investigations is: Somewhat surprisingly, the best-first samples including the most probable diagnoses commonly used in the field proved to be the best choice in a large fraction of the investigated cases. Yet, we also find that, for certain configurations of a diagnosis system, best-first samples imply drastic overheads compared to other sample types. Random samples, though enabling highly reliable estimations, often led to a worse diagnostic efficiency than biased ones. We discuss reasons for this phenomenon and make recommendations which configurations wrt. diagnosis computation algorithm, measurement selection heuristic and sample size users of diagnosis systems should adopt for best diagnostic performance. E.g., best-first samples are favorable for small sample sizes or when the information gain heuristic is used, whereas random ones are best for larger sample sizes. We further reveal that there is a time-information trade-off in diagnosis sampling, i.e., more efficient sampling tends to imply less effective measurements. Finally, we find that an approximate, and often efficient, sampling technique based on the Inv-HS-Tree algorithm (Shchekotykhin et al. 2014) in many cases provides a good trade-off between sampling efficiency and diagnostic effectivity. We believe that these results, especially the recommendations (Sec. 3.7), can be of high value for both diagnosis researchers and practitioners.

⁶Those bullet points marked by a “*” we plan to address in terms of additional experiments as part of future work.

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