

Explanatory Learning: Towards Artificial Scientific Discovery

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Abstract

Explanations are the fuel of progress, the fundamental tool through which humans have increased their agency, earning more and more control over their future throughout history. So far, the production of these special symbolic sequences has been a unique prerogative of humans, who greatly improved the process over the last centuries with the emergence of the scientific method. In this work, we try to formalize this epistemological breakthrough to make it digestible by a machine, with the ultimate goal of building an artificial scientist and breaking the monopoly of humans in producing new explanations. Our Explanatory Learning (EL) construction stands over the Machine Learning field. Unlike traditional AI methods based on human-coded interpreters—such as program synthesis—EL builds upon the notion that a true artificial scientist can only emerge when a machine is capable of autonomously interpreting symbols. Consequently, EL necessitates a learned interpreter, trained on a limited set of raw strings hiding explanations, paired with observations of the corresponding phenomena—akin to a science book written in hieroglyphic. To exemplify the challenges of EL, we present Odeen, a basic environment that simulates a small universe full of phenomena to explain. Finally, we introduce Critical Rationalist Networks, a deep learning approach to EL aligned with the Popperian view of knowledge acquisition. Using Odeen as a testbed, we show how CRNs outperform standard empiricist end-to-end approaches of similar size and architecture (Transformers) in discovering explanations for unseen phenomena.

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Figure 1. The Odeen universe. A convenient setting to study and test the process of knowledge discovery in machines. Like the night sky was for humans. ^{*}Galileo did not sketch negative examples.

1. Introduction

Making accurate predictions about the future is a key ability to survive and thrive in a habitat. Living beings have evolved many systems to this end, such as memory (McCConnell, 1962), and several can predict the course of complex phenomena (Taylor et al., 2012). However, no animal comes even close to the prediction ability of humans, which stems from a unique-in-nature system.

At the core of this system lies an object called *explanation*, formed by the proposition of a language, which has a remarkable property: it can be installed with ease into another human speaking the same language, allowing to make predictions on new phenomena without ever having experienced them. When the installation is successful, we say that the human has *understood* the explanation.

This process is key to the success of human beings. An individual can provide accurate predictions for a multitude of phenomena without going through a painful discovery process for all of them, but only needs an operating system – mastering a language – and someone who communicates the relevant explanations; this way, the individual can focus on unexplained phenomena. When an explanation is found for them, it is added to the existing shared collection, which we call *knowledge*.

How can we make machines take part in this orchestra? With this work, we try to shed new light on this problem. Specifically, we propose a learning procedure to allow machines (i) to *understand* existing explanations, in the sense described above, and (ii) create new explanations for unexplained phenomena, much like human scientists do.

¹The explanation *Four wandering stars having their period*

Our contribution in this sense is threefold:

i) We formulate the challenge of creating a machine that masters a language as the problem of learning an interpreter from a collection of examples in the form *explanation-observations*. The only assumption we make is this dual structure of data; explanations are free strings, and are not required to fit any formal grammar. This results in the *Explanatory Learning* (EL) framework described in Sec. 2.

ii) We present Odeen, a basic environment to test EL approaches, which draws inspiration from the board game Zendo (Heath, 2001). Odeen simulates the work of a scientist in a small universe of simple geometric figures, see Figure 1. We present it in Sec. 3, and will release it upon publication.

iii) We argue that the dominating empiricist ML approaches are not suitable for EL problems. We propose *Critical Rationalist Networks* (CRNs), a family of models designed according to the epistemological philosophy pushed forward by Popper (1935). Although a CRN is implemented using two neural networks, the working hypothesis of such a model does not coincide with the adjustable network parameters, but rather with a language proposition that can only be accepted or refused *in toto*. We will present CRNs in Sec. 4, and test their performance on Odeen in Sec. 5.

2. Explanatory Learning

Humans do not master a language from birth. A baby can not use the message “this soap stings” to predict the burning sensation caused by contact with the substance. Instead, the baby gradually *learns* to interpret such messages and make predictions for an entire universe of phenomena (Schulz et al., 2007). We refer to this state of affairs as *mastering a language*, and we aim to replicate it in a machine as the result of an analogous learning process.

Using a batch of explanations paired with observations of several phenomena, we want to learn an interpreter to make predictions about novel phenomena for which we are given explanations in the same language. Going a step further, we also want to discover these explanations, when all we have is a handful of observations of the novel phenomena. We first describe the problem setup in the sequel, comparing it to existing ML problems; then we detail our approach in Sec. 4.

Problem setup. Formally, let phenomena P_1, P_2, P_3, \dots be subsets of a universe U , which is a large set with no special structure (i.e., all the possible observations $U =$

around a principal star is adapted from the English translation of the Siderus Nuncius (Galilei, 2016 page 9). First sketch on the left is compatible with the rule since the fourth moon can be hidden by one of the other moons or by Jupyter itself.

$\{x_1, \dots, x_z\}$). Over a universe U , one can define a language L as a pair $(\Sigma_L, \mathcal{I}_L)$, where Σ_L is a finite collection of short strings over some alphabet A , with $|\Sigma_L| \gg |A|$, and \mathcal{I}_L is a binary function $\mathcal{I}_L : U \times \Sigma_L \rightarrow \{0, 1\}$, which we call *interpreter*. We say that a phenomenon P_i is **explainable** in a language L if there exists a string $e \in \Sigma_L$ such that, for any $x \in U$, it occurs $\mathcal{I}_L(x, e) = \mathbf{1}_{P_i}(x)$, where $\mathbf{1}_{P_i}(x)$ is the indicator function of P_i . We call the string e an explanation, in the language L , for the phenomenon P_i .

Explainability definition

Our first contribution is the introduction of a new class of machine learning problems, which we refer to as *Explanatory Learning* (EL).

Consider the general problem of making a new prediction for a phenomenon $P_0 \subset U$. In our setting, this is phrased as a binary classification task: given a sample $x' \in U$, establish whether $x' \in P_0$ or not. We are interested in two instances of this problem, with different underlying assumptions:

- **The communication problem: we have an explanation.** We are given an explanation e_0 for P_0 , in an unknown language L . This means that we do not have access to an interpreter \mathcal{I}_L ; e_0 looks like Japanese to a non-Japanese speaker. Instead, we are also given other explanations $\{e_1, \dots, e_n\}$, in the same language, for other phenomena P_1, \dots, P_n , as well as observations of them, i.e., datasets $\{D_1, \dots, D_n\}$ in the form $D_i = \{(x_1, \mathbf{1}_{P_i}(x_1)), \dots, (x_m, \mathbf{1}_{P_i}(x_m))\}$, with $m \ll |U|$. Intuitively, here we expect the learner to use the explanations paired with the observations to build an approximated interpreter $\hat{\mathcal{I}}_L$, and then use it to make the proper prediction for x' by evaluating $\hat{\mathcal{I}}_L(x', e_0)$.
- **The scientist problem: we do not have an explanation.** We are given explanations $\{e_1, \dots, e_n\}$ in an unknown language L for other phenomena P_1, \dots, P_n and observations of them $\{D_1, \dots, D_n\}$. However, we do not have an explanation for P_0 ; instead, we are given just a small set of observations $D_0 = \{(x_1, \mathbf{1}_{P_0}(x_1)), \dots, (x_k, \mathbf{1}_{P_0}(x_k))\}$ and two guarantees, namely that P_0 is explainable in L , and that D_0 is **representative** for P_0 in L . That is, for every phenomenon $P \neq P_0$ explainable in L there should exist at least a $x_i \in D_0$ such that $\mathbf{1}_{P_0}(x_i) \neq \mathbf{1}_P(x_i)$. Again, we expect the learner to build the interpreter $\hat{\mathcal{I}}_L$, which should first guide the search for the missing explanation e_0 based on the clues D_0 , and then provide the final prediction through $\hat{\mathcal{I}}_L(x', e_0)$.

Representativity definition

Several existing works fall within the formalization above. The seminal work of (Angluin, 1987) on learning regular sets is an instance of the scientist problem, where finite automata take the role of explanations, while regular sets

are the phenomena. More recently, CLEVR (Johnson et al., 2017) posed a communication problem in a universe of images of simple solids, where explanations are textual and read like “There is a sphere with the same size as the metal cube”. Another recent example is CLIP (Radford et al., 2021), where 400,000,000 captioned internet images are arranged in a communication problem to train an interpreter, thereby elevating captions to the status of explanations rather than treating them as simple labels². With EL, we aim to offer a unified perspective on these works, making explicit the core problem of learning an interpreter purely from observations.

Relationship with other ML problems. We briefly discuss the relationship between EL and other problems in ML, pointing to Sec. 6 for additional discussion on the related work.

EL can be framed in the general meta-learning framework. The learner gains experience over multiple tasks to improve its general learning algorithm, thus requiring fewer data and less computation on new tasks. However, differently from current meta-learning approaches (Finn et al., 2017; Lee et al., 2019), we are not optimizing for any meta-objective (Hospedales et al., 2020). Instead, we expect the sought generality to be a consequence of implicitly defining an interpreter through a limited set of examples rather than an explicit goal to optimize for.

To many, the concept of explanation may sound close to the concept of program; similarly, the scientist problem may seem a rephrasing of the fundamental problem of Inductive Logic Programming (ILP) (Shapiro, 1981) or Program Synthesis (PS) (Balog et al., 2017). This is not the case. ILP has the analogous goal of producing a hypothesis from positive/negative examples accompanied by background knowledge. Yet, ILP requires observations to be expressed as logic formulas, a task requiring a human; only then the ILP solver outputs an explanation in the form of a logic proposition, which in turn is interpreted by a human expert. With EL, data can be fed as-is without being translated into logic propositions, and a learned interpreter plays the expert’s role. PS also admits raw data as input, it yields a program as output, and replaces the expert with a hand-crafted interpreter; still, the sequence of symbols produced by a PS system only makes sense to a human (who designed the interpreter), not to the system itself. Instead, in EL, the interpreter is learned from data rather than hardcoded. An empirical comparison demonstrating the benefits of EL over PS is given in Sec. 5.

Next we introduce Odeen, an environment and benchmark to experiment with the EL paradigm.

²This shift greatly improved the performance of their model, as discussed in (Radford et al., 2021) Sec. 2.3).

3. Odeen: a puzzle game as Explanatory Learning environment

Single game. The inset shows a typical situation in a game of Odeen. The players look at a set of structures made of simple geometric figures. Each structure is tagged red or green according to a secret rule, and the players’ goal is to guess this rule. In the example, the rule can not possibly be “A structure must contain at least one red square” since the fifth structure on the left does not contain a red square, but respects the rule (green tag). To win the game, a player must prove to know the rule by correctly tagging a large set of new structures³.

Odeen challenge. We can see each game of Odeen as a different phenomenon of a universe, where each element is a sequence of geometric figures. In this universe, players are scientists like Galileo, trying to explain the new phenomenon; see Figure 1. We can phrase the challenge for an Odeen scientist in this way: make correct predictions for a new phenomenon given few observations of it in addition to explanations and observations of some other phenomena. This is the essence of the Odeen Explanatory Learning problem, see Figure 2 (A and B).

- Why do we need explanations and observations from phenomena different from the one of interest? Indeed, we are able to play Odeen from the very first game.

- We are able to do so only because we are already fluent in the Odeen language, which is a subset of English in the above case. We already have and understand all necessary concepts, such as being “at the right of” something, but also being a “square” or “at least”. Otherwise, we would need past explanations and observations to first build this understanding. Before explaining the dynamic of the Jupiter moons, Galileo learned what “Jupiter” is and what does it mean to “have a period around” something from past explanations and examples provided to him by books and teachers.

³The solution of the inset game is at the end of this footnote. Odeen is inspired by the board game Zendo, where players must explicitly guess the rule, known only to a master. In Zendo, players can also experiment by submitting new structures to the master. Solution: At least one square at the right of a red pyramid.

In Odeen, consider the point of view of someone who does *not* speak the language in which the rules are written; an example of this is in the inset, where the secret explanations are given in hieroglyphics rather than English. Such a player would not be able to tag any structure according to the secret rule, even if the latter is given. However, assume the player has been watching several games together with their secret rules. Reasonably, the player will grow an idea of what those strange symbols mean. If the player then wins several Odeen games, it would be strong evidence of mastering the Odeen language.

Problem formulation. Each game of Odeen is a different phenomenon P_i of a universe U whose elements x are sequences of geometric figures. The specific task is to make correct predictions for a new phenomenon P_0 (a new game) given: (i) a few observations D_0 of P_0 (tagged structures), in conjunction with (ii) explanations $\{e_1, \dots, e_n\}$ and observations $\{D_1, \dots, D_n\}$ of other phenomena (other games and their secret rules). More formally:

Let us be given s unexplained phenomena with k observations each, and n explained phenomena with m observations each; let the n phenomena be explained in an unknown language, i.e., e_1, \dots, e_n are plain strings without any interpreter. The task is to make ℓ correct predictions for each of the s unexplained phenomena.

We consider $\ell = 1176$ (1% of structures); $s = 1132$; $k = 32$; $n = 1438$ or 500 ; m ranges from $10K$ to 50 .

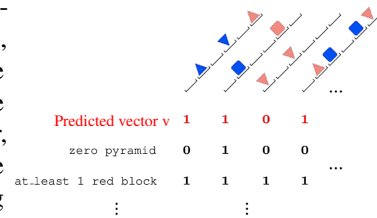
Why not explicitly ask for the rule? Instead of requiring the player to reveal the secret explanation explicitly, we follow the principle of zero-knowledge proofs (Blum et al., 1988). In our setting, this is done by asking the player to correctly tag many unseen structures according to the discovered rule. This makes it possible for any binary classification method to fit our EL environment without generating text. A winning condition is then defined by counting the correct predictions, instead of a textual similarity between predicted and correct explanation, which would require the player to guess word-by-word the secret rule. In fact, different phrasings with the same meaning should grant a victory, e.g., “at least one pyramid pointing up and at most one pyramid pointing up” is a winning guess for the secret rule “exactly one pyramid pointing up”⁴. A brute-force enumeration of all equivalent phrasings, in turn, would not allow solutions like “exactly one *one* pyramid pointing up”, where “one” is mistakenly repeated twice; intuitively, we want to accept

⁴The intuitive notion of meaning adopted here coincides with the pragmatic definition given by Peirce (1878, Sec. II), which identifies the meaning of an expression with the set of all conceivable practical consequences that derive from its acceptance. We refer the reader to *Kant and the Platypus* for a readable discussion of this view (Eco, 2000, Sec. 3.3), involving the first description of horses given by Aztecs.

this as correct and dismiss the grammatical error. Similarly, a solution like “exactly one pointing up”, where “pyramid” is omitted, should be accepted in a universe where only pyramids point up. We will reencounter these examples in Sec. 5 when we discuss the key properties of our approach.

Dataset generation. Odeen structures are sequences of six elements including spaces, blues or reds, squares or pyramids, the latter pointing up or down. The size of the universe is $|U| = 7^6 = 117,649$ possible structures. We further created a small language with objects, attributes, quantifiers, logical conjunctions, and interactions (e.g., “touching”, see Appendix A). The grammar generates $\approx 25k$ valid rules in total. Each of the $|U|$ structures is tagged according to all the rules. The tagging is done by an interpreter implemented via regular expressions.

Metrics. As described above, the task is to tag ℓ new structures for each of s unexplained games. An EL algorithm addressing this task encodes the predicted rule as an ℓ -dimensional binary vector \mathbf{v} per game (predicted vector), where $v_i = 1$ means that the i -th structure satisfies the predicted rule, and $v_i = 0$ otherwise (see inset). Let \mathbf{w}^* be the ground-truth vector, obtained by tagging the ℓ structures according



to the correct secret rule. Then, the Hamming distance $d_H(\mathbf{v}, \mathbf{w}^*)$ measures the number of wrong tags assigned by the EL algorithm; if $d_H(\mathbf{v}, \mathbf{w}^*) < d_H(\mathbf{v}, \mathbf{w}_i)$, where $\mathbf{w}_i \neq \mathbf{w}^*$ ranges over all the possible $\approx 25k$ rules, then the predicted rule \mathbf{v} made by the algorithm is deemed correct.

According to this, the *Nearest Rule Score* (NRS) is the number of correctly predicted rules over a total of s games. A second score, the *Tagging Accuracy* (T-Acc), directly counts the number of correct tags averaged over s games; this is more permissive in the following sense. Consider two different rules A and B sharing 99% of the taggings, and let A be the correct one; if an EL model tags all the structures according to the *wrong* rule B , it still reaches a T-Acc of 99%, but the NRS would be 0. An EL algorithm with these scores would be good at making predictions, but would be based on a wrong explanation.

4. Critical Rationalist Networks

In principle, an EL problem like Odeen can be approached by training an end-to-end neural network to predict $\hat{y} = 1_{P_i}(x')$, given as input a set of observations D_i and a single sample x' (see Figure 2 C, left). Such a model would assume that all the information needed to solve the task is embedded in the data, ignoring the explanations; we may

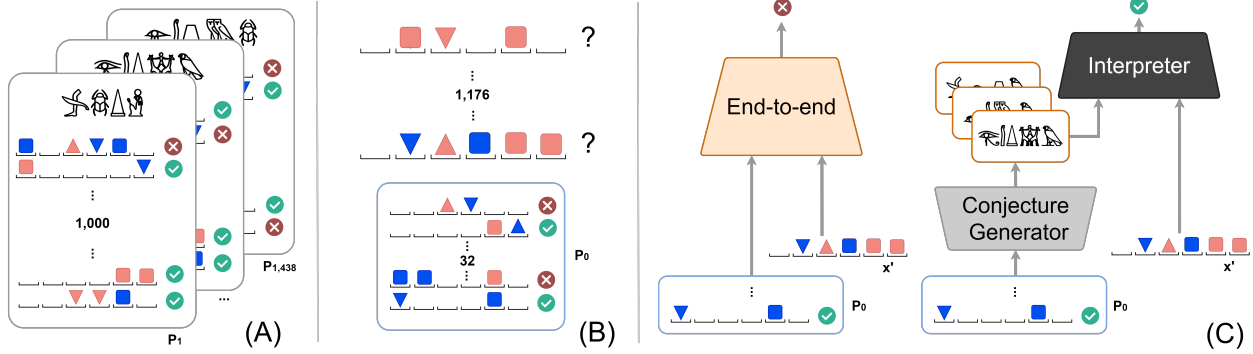


Figure 2. **Odeen Explanatory Learning problem.** Given observations and explanations in an unknown language for some phenomena (A), plus a few observations of a new phenomenon, explain the latter and prove this knowledge by correctly tagging a large set of new samples (B). An empiricist approach attempts to extract this knowledge from data (C, left); a rationalist one conceives data as theory-laden observations, used to find the true explanation among a set of conjectures (C, right).

call it a “radical empiricist” approach (Pearl, 2021). A variant that includes the explanations in the pipeline can be done by adding a textual head to the network. This way, we expect performance to improve because predicting the explanation string can aid the classification task. As we show in the experiments, the latter approach (called “conscious empiricist”) indeed improves upon the former; yet, it treats the explanations as mere data, nothing more than mute strings to match, in a Chinese room fashion (Searle, 1980; Bender & Koller, 2020).

In the following, we introduce a “rationalist” approach to solve EL problems. This approach recognizes the given explanations as existing knowledge, and focuses on interpreting them. Here theory comes first, while the data become theory-laden observations.

Learning model. Our *Critical Rationalist Networks* (CRNs) tackle the EL scientist problem introduced in Sec. 2 to find $y = \mathbf{1}_{P_0}(x')$ given x' , D_0 , $\{D_1, \dots, D_n\}$, $\{e_1, \dots, e_n\}$. They are formed by two independently trained models:

(i) A stochastic *Conjecture Generator*

$$\mathcal{CG} : \{(x, \mathbf{1}_P(x))_{j=1}^k\} \mapsto e,$$

taking $k \leq |D_0|$ pairs $(x, \mathbf{1}_P(x)) \in D_i$ as input, and returning an explanation string $e \in \Sigma$ as output. \mathcal{CG} is trained to maximize the probability that $\mathcal{CG}(D_i) = e_i$ for all $i = 1, \dots, n$, where $D_i \subset D_0$ is a random sampling of D_0 , and $|D_i| = k$.

(ii) A learned *Interpreter*

$$\mathcal{I} : (e, x) \mapsto \hat{y},$$

which takes as input a string $e \in \Sigma$ and a sample $x \in U$, to output a prediction $\hat{y} \in \{0, 1\}$. \mathcal{I} is trained to maximize the probability that $\mathcal{I}(e_i, x) = \mathbf{1}_{P_i}(x)$, with $i = 1, \dots, n$ and $(x, \mathbf{1}_{P_i}(x)) \in D_i$.

At test time, we are given a trained \mathcal{CG} and a trained \mathcal{I} , and we must predict whether some $x' \notin D_0$ belongs to P_0 or not.

The idea is to first generate t conjectures by applying \mathcal{CG} t times to the dataset D_0 ; then, each conjecture is verified by counting how many times the interpreter \mathcal{I} outputs a correct prediction over D_0 . The conjecture with the highest hit rate is our candidate explanation \hat{e}_0 for P_0 . Finally, we obtain the prediction \hat{y}' as $\mathcal{I}(\hat{e}_0, x')$. See Figure 3 (left) for a step-by-step pseudo code.

Remarks. The interpreter \mathcal{I} is a crucial component of our approach. A poor \mathcal{I} may fail to identify e_0 among the generated conjectures, or yield a wrong prediction y' when given the correct e_0 . On the other hand, we can work with a \mathcal{CG} of any quality and safely return as output an *unknown* token, rather than a wrong prediction, whenever e_0 does not appear among the generated conjectures. The role of \mathcal{CG} is to trade-off performance for computational cost, and is controlled by the parameter t . Larger values for t imply more generated conjectures, corresponding to exhaustive search if taken to the limit (as done, e.g., in Radford et al. (2021)). This potential asymmetry in quality between \mathcal{CG} and \mathcal{I} is tolerated, since the learning problem solved by \mathcal{CG} is generally harder.

Secondly, although a CRN is implemented using neural networks, as we shall see shortly, its working hypothesis does not coincide with a snapshot of the countless network’s parameters; rather, the working hypothesis is but the small conjecture analyzed at a given moment. This way, the CRN hypothesis is detached from the model and can only be accepted or refused in its entirety, rather than being slightly adjusted at each new data sample (Figure 2C, the hypotheses are in orange).

Implementation. Figure 3 (right) illustrates the architecture of CRNs, which we implement using encoder-decoder transformers (Vaswani et al., 2017). The figure also shows the architecture of the baseline methods EMP-R and EMP-C, corresponding to the end-to-end NN model and its variant with a textual head, respectively. We refer to the Appendix for further details.

Input: dataset D_0 , sample x'
Output: explanation \hat{e}_0 , prediction \hat{y}'
 $C \leftarrow \emptyset$
while $|C| < t$ **do**
 $\tilde{D}_0 \leftarrow$ random pairs $\subset D_0$
 $C \leftarrow C \cup \mathcal{CG}(\tilde{D}_0)$ } generate conjectures
end
 $\{s_i \leftarrow 0\}$ for $i = 1, \dots, t$
for $j = 1, \dots, k$ **do**
 $(x, y) \leftarrow$ random $\in D_0$
 for $i = 1, \dots, t$ **do**
 $\hat{y} \leftarrow \mathcal{I}(c_i \in C, x)$
 if $\hat{y} = y$ **then**
 $s_i \leftarrow s_i + 1$
 end
 end } verify conjectures
end
 $\ell \leftarrow \arg \max_i \{s_i\}$
 $\hat{e}_0 \leftarrow c_\ell \in C$
 $\hat{y}' \leftarrow \mathcal{I}(\hat{e}_0, x')$

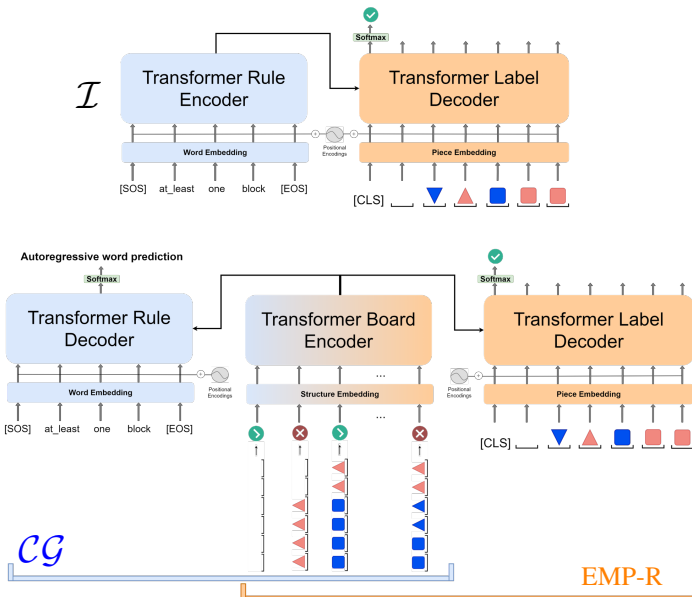


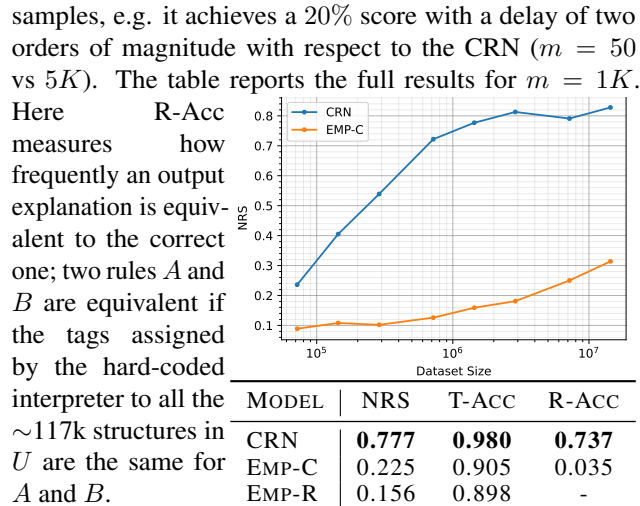
Figure 3. **Left:** Test-time algorithm of CRNs. **Right:** CRNs are implemented using encoder-decoder transformers blocks, details of the parameters in Appendix B. **Right-top:** \mathcal{I} denotes the interpreter model (rule encoder and label decoder). **Right-bottom:** The conjecture generator \mathcal{CG} is composed by blue blocks. The “radical empiricist” (EMP-R) is composed by orange blocks. The “conscious empiricist” (EMP-C) baseline model consists of all the transformer blocks in the right-bottom figure, board encoder with rule and label decoders.

5. Experiments

We extensively compared CRNs to the radical (EMP-R) and conscious (EMP-C) empiricist models over the Odeen EL problem, and analyzed several fundamental aspects.

Generalization power and data scaling laws. Seeing the generalization power of a learning algorithm as its ability in discovering new knowledge from little data, the Odeen challenge asks to explain 1132 unknown phenomena for which only 32 observations are available. We measure the performance on this task through a proof of knowledge based on the successful tagging of 1176 new structures per phenomenon (NRS). The information available at training time consists of symbolic explanations from 1438 known phenomena paired with m observations each (see Fig. 2A), we evaluated several settings with m ranging from 10K to 50. No test explanation is equivalent to the ones seen at training. An important example is the bigram “exactly two”, which appears in the test set, but was deliberately excluded from training; the training rules only contain “at least/most two” and “exactly one”. With $m = 1K$, the CRN guessed 40% of the 72 test rules with “exactly two”, while the empiricist models only 4% (EMP-C) and 0% (EMP-R). Some example games can be found in Appendix D.

The plot in the inset shows the NRS trends for the CRN and EMP-C over different sizes of the training dataset. Despite the EMP-C and CRN have approximately the same number of learnable parameters ($\approx 6M$), the CRN performance grows faster and earlier as data scales. The EMP-C barely improves before training at least on 1 million



As expected, the explanation predicted by the conscious empiricist model is rarely correct (R-Acc 3.5%), even when it tags some structures properly (NRS 22.5%); indeed, EMP-C gives no guarantee for the predicted explanation to be consistent with the tags prediction. Conversely, the CRN consistently provides the correct explanation when it is able to properly tag the new structures (NRS 77.7%, R-Acc 73.7%). The 4% gap between the two scores is clarified in the next paragraph.

Handling ambiguity and contradiction. One may reasonably expect that a CRN equipped with the ground-truth interpreter used to generate the dataset, would perform better than a CRN with a learned interpreter. Remarkably, this is not always the case, as reported in Table 1.

Table 1. **Explanatory Learning vs Program Synthesis paradigm.** Performance comparison of a data-driven vs ground-truth interpreter in a CRN. The last column shows the tag prediction accuracy of the learned \mathcal{I} , when provided with the correct rule.

TRAIN DATA		NRS		T-ACC LEARNED \mathcal{I}
		FULLY-LEARNED CRN	HARDCODED \mathcal{I} CRN	
10K STRUCT.	1438 RULES	0.813	0.801	0.997
1K STRUCT.	1438 RULES	0.777	0.754	1.000
100 STRUCT.	1438 RULES	0.402	0.406	0.987
10K STRUCT.	500 RULES	0.354	0.377	0.923
1K STRUCT.	500 RULES	0.319	0.336	0.924
100 STRUCT.	500 RULES	0.109	0.101	0.920

The better performance of the fully learned interpreter over the ground-truth one is due to its ability to process ill-formed conjectures generated by the \mathcal{CG} . The conjecture “at least one pointing up” makes the hard-coded interpreter fail, since “pointing up” must always follow the word “pyramid” by the grammar. Yet, in Odeen, pyramids are the only objects that point, and the learned \mathcal{I} interprets the conjecture correctly. Other examples include: “exactly one red block touching pyramid blue” (“pyramid” and “blue” are swapped), or the contradictory “at least one two pyramid pointing up and exactly one red pyramid”, which was interpreted correctly by ignoring the first “one”. When the learned interpreter is not very accurate, the effect of errors in tagging prevails.

Making sense out of ambiguous or contradictory messages⁵ is a crucial difference between a learned interpreter vs a hardcoded one. As Rota (1991) reminds us, a concept does not need to be precisely defined in order to be meaningful. Our everyday reasoning is not precise, yet it is effective. “After the small tower, turn right”; we will probably reach our destination, even when our best attempts at defining “tower”, as found, e.g., in the Cambridge dictionary, begin with “a tall, narrow structure...”.

Explainability. The predictions of a CRN are *directly caused* by a human-understandable explanation that is available in the output; this makes CRNs explainable by construction. Further, CRNs allow counterfactuals; one may deliberately change the output explanation with a new one to obtain a new prediction. The bank ML algorithm spoke: “Loan denied”; explanation: “Two not paid loan in the past and resident in a district with a high rate of insolvents”. With a CRN, we can easily discard this explanation and compute a new prediction for just “Two not paid loan in the past”.

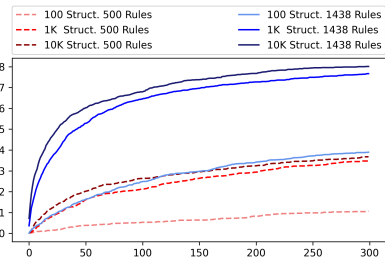
Importantly, by choosing a training set, we control the language used for explanations; i.e., we explicit the biases that will steer the learning of generalizations (Mitchell, 1980). This allows a CRN to ignore undesirable patterns in the data (e.g., skin color) if these can not be expressed in the

⁵This is one of seven essential abilities for intelligence as found in *GEB* (Hofstadter, 1979, Introduction).

chosen language. If the Odeen training set had no rule with “pointing up/down”, the learned interpreter would see all equal pyramids, even with unbalanced training data where 90% of pyramids point up.

On the contrary, current explainability approaches for NNs (end-to-end empiricist models) either require some form of reverse engineering, e.g., by making sense out of neuron activations (Goh et al., 2021), or introduce an ad-hoc block to generate an explanation *given* the prediction, without establishing a cause-effect link between the two (Hendricks et al., 2016; Hind et al., 2019). This practice produces explanations that are not reliable and can be misleading (Rudin, 2019), on the contrary CRNs’ explanations are faithful to what the model actually computes.

Adjustable thinking time. End-to-end models do not exhibit a parameter to adjust their processing to the complexity of the incoming prediction. By contrast, CRNs have a test-time parameter t , corresponding to the number of generated conjectures, which trades off computational cost for performance. In



the inset, we plot the cumulative R-Acc score (y axis) against the number t of generated conjectures (x axis). The curves show that $> 60\%$ of correct explanations are found within the first 50 candidates, and $> 80\%$ are within the first 300. As a reference, a brute force exhaustive search would reach 100% over a search space of 24, 794 possible explanations.

Prediction confidence. As explained in Sec. 4, at test time the CRN selects the conjecture with the highest hit rate among the ones generated by the \mathcal{CG} . Alternatively, one may keep only the conjectures coherent with *all* the structures in the table, returning an “unknown explanation” signal if no such conjectures are found. If the interpreter is sufficiently accurate, this stricter condition barely deteriorates the CRN

performance, and it will never return a prediction based on a possibly wrong explanation. For example, tested in a setting with $n = 1438$, $m = 1000$ (same as the *Generalization power* paragraph), this stricter CRN discovers the correct explanation for 861 out of 1132 new phenomena (76%), and admits its ignorance on the other 271. Conversely, evaluating the confidence of an end-to-end neural network remains an open problem (Meinke & Hein, 2019).

6. Related Work

Epistemology. The deep learning model we propose in this work, CRNs, is designed according to the epistemological theory of critical rationalism advanced by Popper (1935), where knowledge derives primarily from conjectures, criticized at a later stage using data. Deutsch (2011) remarks that to make this critique effective, conjectures should not be adjustable but can only be kept or rejected at each new data sample, as done in CRNs at test time. Only in this way we can discover explanations with “reach”, namely that maintain predictive power in novel situations.

Machine learning. Explanatory Learning enriches the fundamental problem of modern program synthesis (Balog et al., 2017; Sun et al., 2018; Ellis et al., 2020) by including the interpretation step among what should be learned. As seen in the *Handling ambiguity* paragraph, a learned \mathcal{I} can grant better performance by exploiting the ambiguity of language to impose new meaning on arbitrary substrates, which Santoro et al. (2021) recognize as a fundamental trait of symbolic behavior.

Despite the similar underlying motivation, EL fundamentally differs from current meta learning approaches (Weng, 2018), since it does not prescribe any parameter adaptation at test time. In this sense, EL resembles more the Domain Generalization setting, which involves designing a specific model that is robust to domain shift (Li et al., 2018). Unlike DG, EL requires labels to be symbolic sequences rather than a single symbol, but makes no assumption of identical labels between training and test domains⁶. EL requires just that all symbols present in the test sequences are seen at training. While current SOTA approaches in DG do not significantly outperform Empirical Risk Minimization (Gulrajani & Lopez-Paz, 2020), in the EL setting CRNs overcome the performance of standard ERM (EMP-C) by a large margin. Recent literature finds few yet remarkable approaches that fit our EL paradigm, such as CLIP (Radford et al., 2021) in the vision area, and Generate & Rank (Shen et al., 2021) for Math Word Problems in NLP.

The Odeen challenge continues the tradition of AI benchmarks set in idealized domains (Mitchell, 2021). Unlike

⁶The DG version of the Odeen test set would contain the same rules of the training set, changing just the accompanying structures.

CLEVR (Johnson et al., 2017) and ShapeWorld (Kuhnlé & Copestake, 2017), Odeen focuses on abduction rather than deduction. Unlike ARC (Chollet, 2019), Odeen is a closed environment providing all it takes to learn the language needed to solve it. Unlike the ShapeWorld adaptation of Andreas et al. (2017), its score is measured in terms of discovered explanations rather than sparse guessed predictions; further, the test and training set do not share any phenomenon.

Learning theory. Finally, we point out that the expression *Explanatory Learning* was previously used by Aaronson (2013, Sec. 7) to argue about the necessity of a learning theory that models “predictions about phenomena different in kind from anything observed”. The author pointed to the work of Angluin (1987), who generalized the PAC learning model by moving the goal from successful predictions to comprehensive explanations.

7. Conclusions

Recently, the attention on the epistemological foundations of deep learning has been growing. The century-old debate between empiricists and rationalists about the source of knowledge persists, with two Turing prizes on opposite sides; LeCun (2019) argues that empiricism still offers a fruitful research agenda for deep learning, while Pearl (2021) supports a rationalist steering to embrace model-based science principles. This new debate is relevant, since as Pearl notes, today we can submit the balance between empiricism and innateness to experimental evaluation on digital machines.

Limitations and future directions. EL models the essential part of the knowledge acquisition process, namely the interval that turns a mute sequence of symbols into an explanation with reach. However, our modeling assumes a representative set of observations D_0 to be given (the $k = 32$ structures of the new phenomenon). A more comprehensive explanatory model would allow the player to do without these observations, including an interaction phase with the environment where the D_0 itself is actively discovered. We see this as an exciting direction for follow-ups.

Finally, we expect CRNs to be more resilient than end-to-end models to adversarial attacks. For a given data point $x' \in P_0$ classified correctly by an empiricist model, a small adversarial change on D_0 can flip the prediction for x' while remaining unnoticed. Conversely, suppose that a CRN made the prediction for x' , and assume that the correct explanation was ranked as the 5th most likely by the \mathcal{CG} . The same attack on D_0 will have the effect of moving the correct explanation lower in the ranking; however, as long as it stays within the first t conjectures (300 in this paper), it will always be found by the interpreter as the correct solution.

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Appendix

A. Further details on the Odeen⁶ dataset

Training set. The total number of rules produced by the Odeen grammar is 24,794. We consider training sets varying from 500 to 1438 rules. We choose these rules such that each token and each syntactic construct appears at least once; then, we uniformly select the others from the distribution. We removed from the training set any rule containing the bigram `exactly 2`, as well as any rule of the form `at_least 2 X` and `at_most 2 X`, equivalent to `exactly 2 X`. Each rule is associated with a set of 100, 1,000, or 10,000 labelled structures that unambiguously identify a rule equivalence class.

Test set. We generate the 1,132 games that compose the test set the same way, with the additional constraint of excluding the rules belonging to an equivalence class that is already in the training set. In the test set 72 rules contain the bigram `exactly 2`. Rules in the test set are associated with just 32 labelled structures. The first 10 structures are chosen by searching pairs of similar structures with different labels, following a common human strategy in Zendo. The remaining 22 structures are selected to ensure the lack of ambiguity on the board.

Formal definition of the Odeen grammar. The context-free grammar in Figure 4 defines all the acceptable rules in Odeen. This grammar only formalizes which rules are *syntactically correct*. Token names (e.g. `red`, `1` or `touching`) do not imply any rule meaning.

The hard-coded interpreter formalizes how to interpret the rules. Similarly to compilers, it tokenizes and transforms the rule into an abstract syntax tree (AST). The interpreter then adds semantic information to the AST, establishing the truth value of each node based on the truth value of its children and the structure under evaluation.

The Odeen binary semantic representations. By simulating the process of scientific discovery, Odeen offers a convenient simulation of a world described by a language. Besides the computational tractability, the simplicity and adjustable size of the Odeen world allows us to explicit the whole semantics of its language.

This semantics can be encoded in a binary *semantic matrix* S with the 24,794 rules e_i on the rows and the 117,649 structures x_j on the columns. The s_{ij} element of this matrix is equal to 1 if the structure x_j complies with the rule e_i and 0 otherwise, see inset in Section 3, Metrics paragraph. S_{i*} ,

the 117,649-dimensional binary vector coinciding with the i -th row of S , fully represents the meaning of rule e_i in the Odeen world. Similarly, each structure x_j is represented by the 24,794-dimensional binary vector coinciding with the column S_{*j} of S .

In Figure 5, we analyze the distribution of the Hamming weights (i.e., the number of ones) in $\{S_{i*}\}_{i=1}^{117,649}$ (5a) and $\{S_{*j}\}_{j=1}^{24,794}$ (5b). We observe an asymmetry between the rule and structure distributions. On one hand, the semantic representation of a rule can be quite unbalanced, with populated extremes of rules evaluating *all* structures with 1 (or 0) as shown in Figure 5a. On the other hand, Figure 5b shows that the semantic representations of structures are very balanced; most of them have around half zeros and half ones, with no structure with less than 10k or more than 14k ones.

This balanced trend, along with the well separable PCA of $\{S_{*j}\}_{j=1}^{24,794}$ (Figure 6a) suggests that the chosen language produce representations that are effective in separating structures. Conversely, the PCA of $\{S_{i*}\}_{i=1}^{117,649}$ is much less homogeneous (Figure 6b). Here we can recognize two poles, corresponding respectively to rules with all ones and all zeros. We believe that this analysis of the binary semantic representations is only partial, and we leave further exploration for follow-up work.

B. Implementation Details

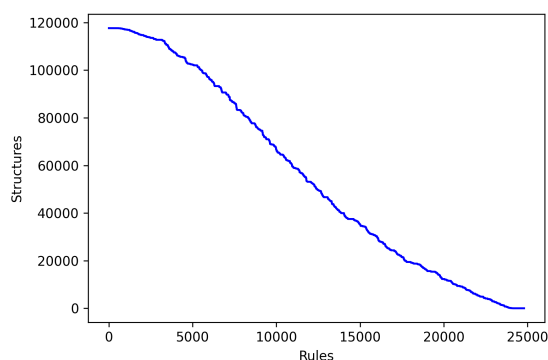
In this paragraph, we give the implementation details of the models proposed and depicted in Figure 3 (right). All the models are based on a Transformer block composed of 4 layers and 8 heads. We used a hidden dimension of 256 for all the models except for the interpreter, where we used a hidden dimension of 128. The models differ primarily by the type of transformer block used (encoder/decoder), inputs and embeddings. In detail:

- **TRANSFORMER LABEL DECODER.** This is a transformer block used to predict a label given a structure. The input structure is a sequence of six learned embeddings, one per piece. We add a sinusoidal positional encoding to each embedding as in the original transformer implementation. The embedding size is 128 in the \mathcal{I} and 256 in the Empiricist models (EMP-C, EMP-R). We used the standard transformer encoder block and added a special token [CLS] at the beginning of the structure like in (Devlin et al., 2019) to perform the classification task.
- **TRANSFORMER RULE DECODER.** This is a transformer decoder block with embedding size of 128 and sinusoidal positional encoding. This decoder block is used to generate the rule by the EMP-C and \mathcal{CG} models.

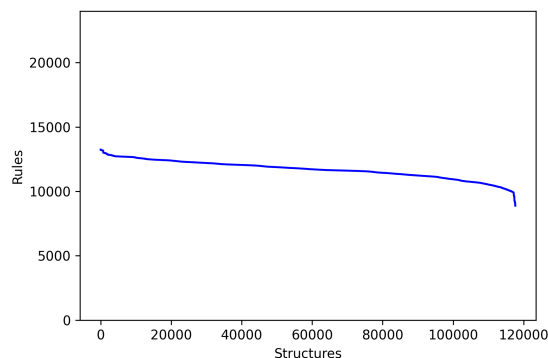
⁶Odeen is the Rational alien in *The Gods Themselves* (1972), a novel by Isaac Asimov about a conspiracy against Earth by the inhabitants of a parallel universe with different physical laws.

$\langle \text{RULE} \rangle$	\models	$\langle \text{PROP_S} \rangle \mid \langle \text{PROP} \rangle \mid \langle \text{PROP_S} \rangle \langle \text{CONJ} \rangle \langle \text{PROP_S} \rangle$
$\langle \text{PROP} \rangle$	\models	$\langle \text{QTY} \rangle \langle \text{OBJ} \rangle \langle \text{REL} \rangle \langle \text{OBJ} \rangle$
$\langle \text{PROP_S} \rangle$	\models	$\langle \text{QTY} \rangle \langle \text{OBJ} \rangle$
$\langle \text{OBJ} \rangle$	\models	$\langle \text{COL} \rangle \mid \langle \text{SHAPE} \rangle \mid \langle \text{COL} \rangle \langle \text{SHAPE} \rangle$
$\langle \text{QTY} \rangle$	\models	$\text{at_least} \langle \text{NUM} \rangle \mid \text{exactly} \langle \text{NUM} \rangle \mid \text{at_most} \langle \text{NUM} \rangle \mid \text{zero}$
$\langle \text{SHAPE} \rangle$	\models	$\text{pyramid} \langle \text{ORIEN} \rangle \mid \text{pyramid} \mid \text{block}$
$\langle \text{REL} \rangle$	\models	$\text{touching} \mid \text{surrounded_by} \mid \text{at_the_right_of}$
$\langle \text{ORIEN} \rangle$	\models	$\text{pointing_up} \mid \text{pointing_down}$
$\langle \text{NUM} \rangle$	\models	$1 \mid 2$
$\langle \text{CONJ} \rangle$	\models	$\text{and} \mid \text{or}$
$\langle \text{COL} \rangle$	\models	$\text{red} \mid \text{blue}$

Figure 4: Grammar productions for the Odeen Language.



(a)



(b)

Figure 5: Hamming weight of the binary semantic representation of each rule (a) and each structure (b). We sort them in descending order for visualization purposes.

- **TRANSFORMER BOARD ENCODER.** This is a transformer encoder block used to encode the (structure, label) pairs. The input is encoded a sequence of 32 learned embeddings, one per structure-label pair.

The size of each embedding is 256. We did not add positional encodings, since the specific position of structure-label pairs among the 32 is not relevant. This block is used in all the models.

- **TRANSFORMER RULE ENCODER.** This transformer encoder block is used in \mathcal{I} to encode the rule. Its implementation is analogous to the TRANSFORMER RULE DECODER, with the only difference that it does not use causal attention since it is an encoder layer.

Table 2: Number of training epochs for each training regimen.

TRAINING REGIMEN		NUMBER OF EPOCHS
10K STRUCT.	1438 RULES	2
1K STRUCT.	1438 RULES	20
100 STRUCT.	1438 RULES	200
10K STRUCT.	500 RULES	6
1K STRUCT.	500 RULES	58
100 STRUCT.	500 RULES	576

Training Procedure. All the models are trained with a learning rate of $3 \cdot 10^{-4}$ using Adam (Kingma & Ba, 2017), a batch size of 512 and early-stop and dropout set to 0.1 to prevent overfitting. We train all the models on randomly sampled sets of 32 (structure, label) pairs to prevent overfitting on specific boards. Table 2 describes the number of epochs for each training regimen. Models are trained to: predict the label of a structure given the board (EMP-R); predict the label of a structure given the 32 pairs (structure, label) and the associated rule (EMP-C); predict the rule given the 32 pairs ($\mathcal{C}\mathcal{G}$); predict the label of a structure given a rule (\mathcal{I}).

Where $300 \cdot \mathcal{CG}$ stands for the 300 beams used to get 300 conjectures from the conjecture generator \mathcal{CG} . Each conjecture (300) is then tested on all the board structures (b) by the interpreter \mathcal{I} . Finally \mathcal{I} is called to apply the chosen conjecture on each new structure (s). As an upper bound, an exhaustive search algorithm (EXV SRC) uses no conjecture generator, and thus has to evaluate with \mathcal{I} all admissible rules (r) on each structure of the board. Conversely, the empiricist approach provide label predictions through a single end-to-end model which is simply called s times. Concerning the problem of inferring explicitly the textual rule, using more beams in the empiricists models does not provide any increase in performance, i.e. the true rule is not a more probable proposition accessible through a larger beam search.

We measured also the absolute time in seconds with the following hardware configuration for all the experiments: 1 single core hyper threaded Xeon CPU Processor with 2.2 Ghz, 2 threads; 12.7 GiB. of RAM; a Tesla T4 GPU, with 320 Turing Tensor Core, 2,560 NVIDIA CUDA cores, and 15.7 GDDR6 GiB of VRAM.

Table 4: Computational cost of our models at test time to tag s new structures. In Odeen $r=24,794$, $b=32$, $s=1,176$. Notice how CRNs offer a good balance between computational efficiency and performance, this trade-off is regulated by a single parameter, the number of beams.

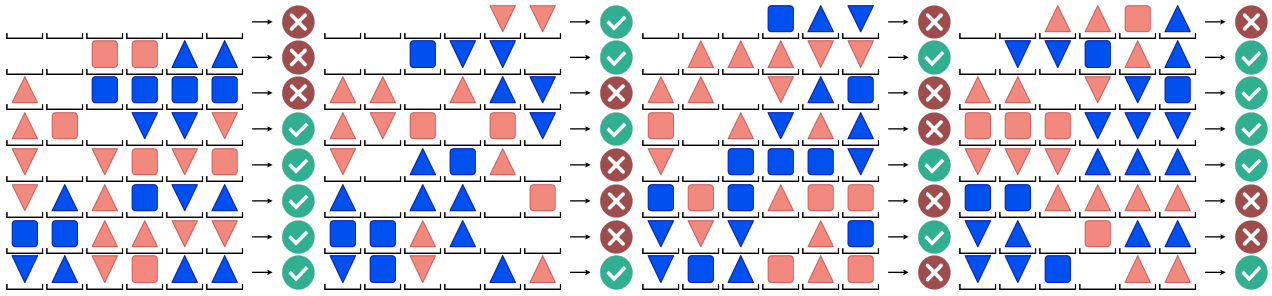
MODEL	COMPUTATIONAL COST	T (s)	NRS
EXV SRC	$r \cdot b \cdot \mathcal{I} + s \cdot \mathcal{I}$	47.9	0.99
CRN [300B]	$300 \cdot \mathcal{CG} + 300 \cdot b \cdot \mathcal{I} + s \cdot \mathcal{I}$	0.79	0.81
CRN [10B]	$10 \cdot \mathcal{CG} + 10 \cdot b \cdot \mathcal{I} + s \cdot \mathcal{I}$	0.43	0.35
EMP	$s \cdot \text{EMP-R}$	0.15	0.35

Table 5: Computational cost of our models at test time to produce the textual rule in output

MODEL	COMPUTATIONAL COST	T (s)	R-ACC
EXV SRC	$r \cdot b \cdot \mathcal{I}$	47.8	0.99
CRN [300B]	$300 \cdot \mathcal{CG} + 300 \cdot b \cdot \mathcal{I}$	0.72	0.77
CRN [10B]	$10 \cdot \mathcal{CG} + 10 \cdot b \cdot \mathcal{I}$	0.35	0.35
EMP [300B]	300· EMP-C	0.41	0.07
EMP [10B]	10· EMP-C	0.10	0.07
EMP [1B]	1· EMP-C	0.10	0.07

D. Odeen example games

In the following pages we propose a collection of qualitative results showing a series of Odeen games from the test set and how they are solved by the proposed models. For each model, we report the predicted rule (only for EMP-C and the CRN), the accuracy on the structures labeling (T-acc), and a mark that indicates whether the nearest rule is the correct one (NRS). All the models are trained on 1,438 rules with 1,000 structures per rule.



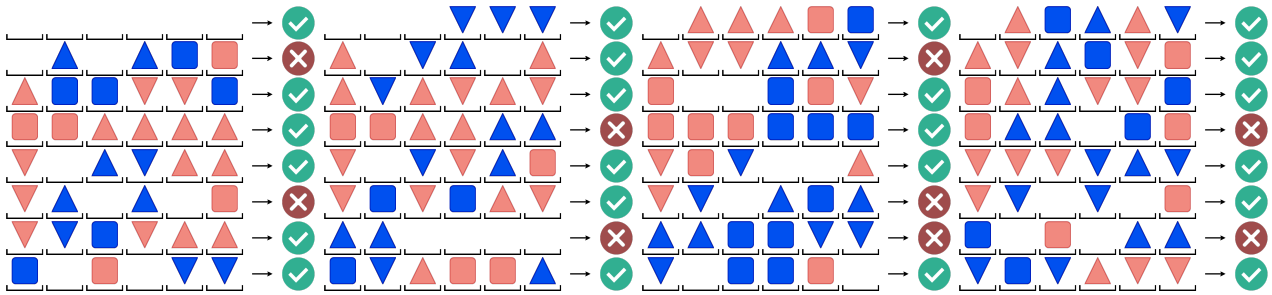
Board 01

Golden Rule: “at_least 2 pyramid pointing_down”

CRN: “at_least 2 pyramid pointing_down”; T-acc 1.0 ✓

EMP-C: “at_least 1 pyramid touching touching”; T-acc: 0.76 ✗

EMP-R: T-acc 0.72 ✗



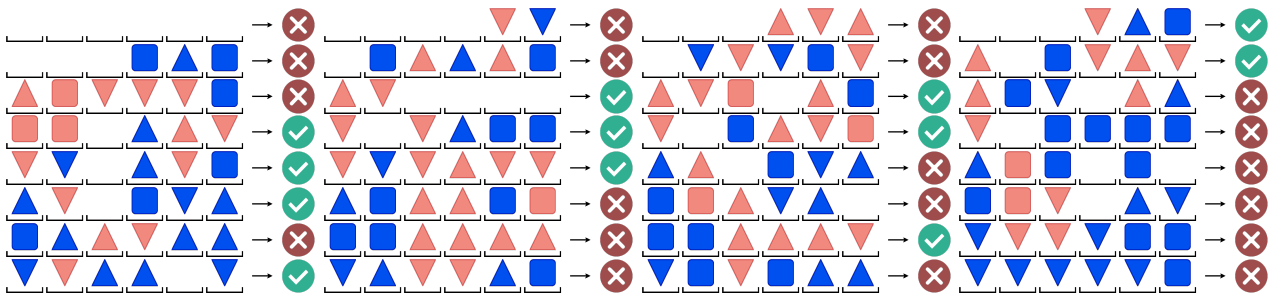
Board 04

Golden Rule: “at_most 1 blue pyramid pointing_up”

CRN: “zero blue or at_most 1 blue pyramid pointing_up”; T-acc 1.0 ✓

EMP-C: “zero 1 blue touching or or”; T-acc: 0.89 ✗

EMP-R: T-acc 0.92 ✓



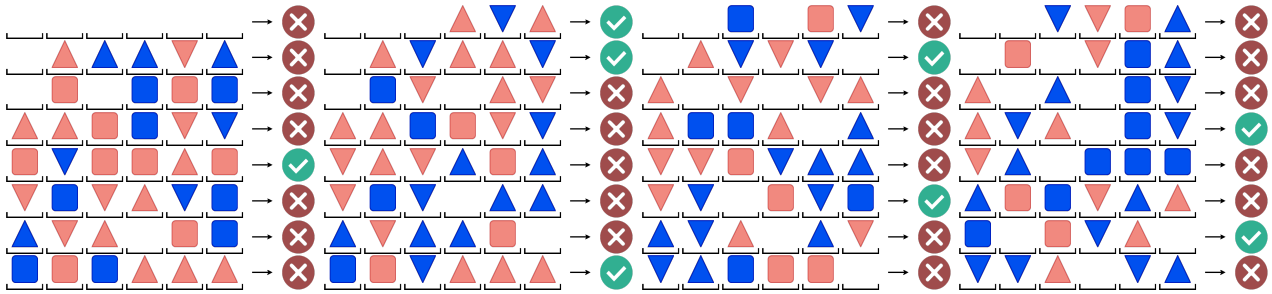
Board 09

Golden rule: “exactly 1 pyramid pointing_up touching red pyramid pointing_down”

CRN: “exactly 1 red pyramid pointing_down touching pyramid pointing_up”, T-acc 0.95 ✗

EMP-C: “exactly 1 red at_the_right_of and red”, T-acc: 0.80 ✗

EMP-R: T-acc 0.79 ✗



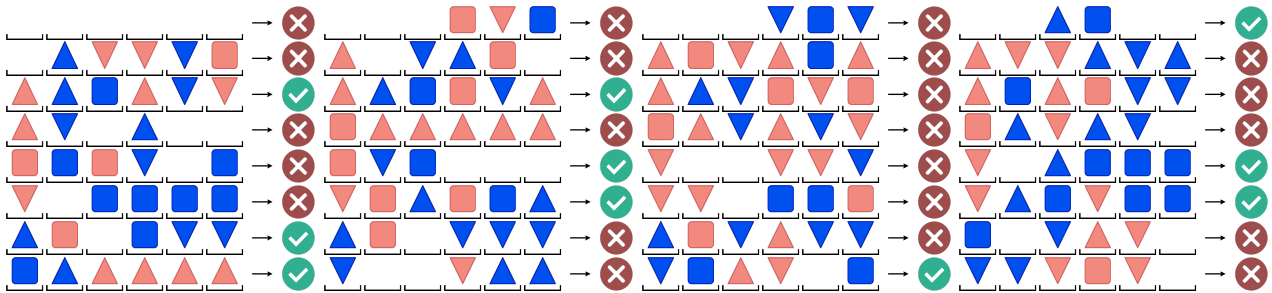
Board 25

Golden rule: "at least 2 red touching blue pyramid pointing down"

CRN: "at least 2 red touching blue pyramid pointing down", T-acc 1.0 ✓

EMP-C: "at least 2 red touching blue pyramid", T-acc: 0.87 ✗

EMP-R: T-acc 0.69 ✗



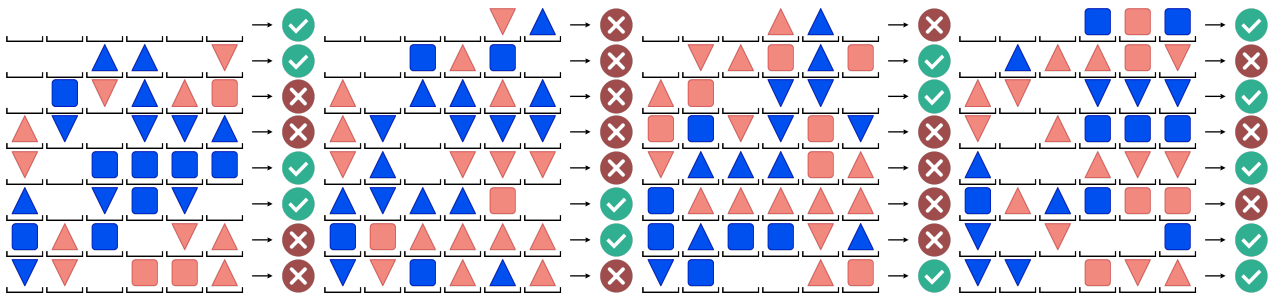
Board 30

Golden rule: "exactly 1 blue pyramid touching blue block"

CRN: "exactly 1 blue pyramid touching blue block", T-acc 1.0 ✓

EMP-C: "exactly 1 blue pyramid touching block block", T-acc: 0.97 ✓

EMP-R: T-acc 0.79 ✗



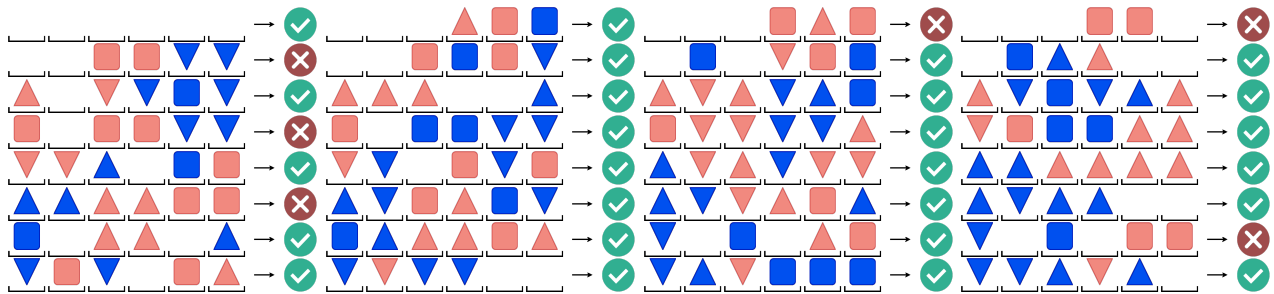
Board 75

Golden rule: "zero blue touching red pyramid"

CRN: "zero blue touching red pyramid", T-acc 1.0 ✓

EMP-C: "zero blue touching red", T-acc: 0.85 ✗

EMP-R: T-acc 0.91 ✓



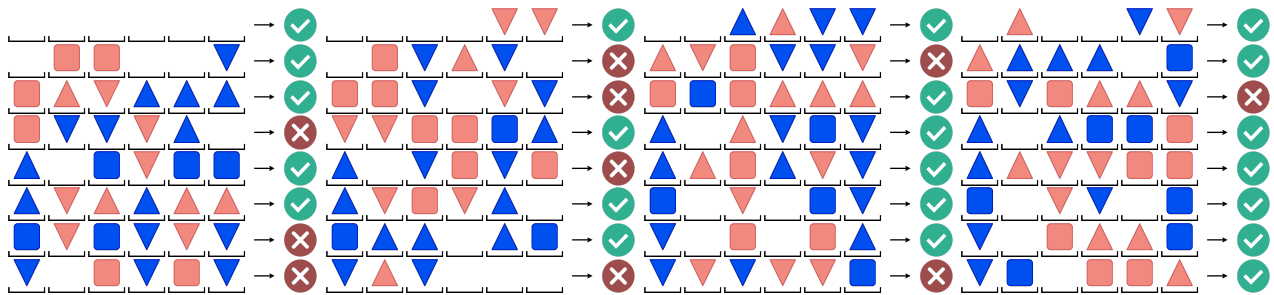
Board 97

Golden rule: "at_most 1 red block touching red"

CRN: "at_most 1 red block touching red", T-acc 1.0 ✓

EMP-C: "at_most 1 red touching at_the_right_of red", T-acc: 0.98 ✓

EMP-R: T-acc 0.93 ✗



Board 103

Golden rule: "at_most 1 blue pyramid pointing_down touching red"

CRN: "at_most 1 blue pyramid pointing_down touching red", T-acc 1.0 ✓

EMP-C: "at_most 1 blue pyramid pointing_down touching red", T-acc: 0.98 ✓

EMP-R: T-acc 0.85 ✗