Heuristic Search Using Language Models and Reinforcement Learning

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***Abstract*—This article extends the applicability domain of language models to problems where candidate solutions can be expressed as an encoded integer sequence. Considering this sequence, language models can operate in the neural machine translation setting and leverage their optimization power for heuristic search techniques. Reinforcement Learning (RL) is applied to Language Models (LM), regardless of whether character-level or word-level models are used as a basis. To stabilize the learning, several approaches are explored, including functional and architectural decoupling. The framework is then applied to two combinatorial problems, namely the Traveling Salesman Problem benchmark and Neural Architecture Search, which is used to generate a hierarchical (tree-based) text classifier where the blocks are inspired by the InceptionV1 architecture. The decoupling results are the main contribution of this paper, easing the RL and LM stabilization requirements while expanding the resolution domain beyond Markov Decision Processes to non-causal normative heuristic problems, such as Neural Architecture Search (NAS).**

Keywords-Heuristic Optimization; Reinforcement Leaning; Language Model; Task Semantic Segmentation; Artificial Neural Network.

I. Introduction

Regarding the Natural Language Processing domain, the auto-encoder Language Models are typically trained on a large corpus. To evaluate the language model, the pretrained encoder, along with a custom decoder tailored to the downstream task, is then fine-tuned to address the specific task. The encoder part of the language model retains knowledge and maps semantics to a reduced latent dimension. This learned mapping keeps, in the encoder's weights, general type features, such as how to speak a language. This work explores the language model's encoder capability to retain the semantics of other problems beyond merely speaking a language. Additionally, the generative capability of language models is examined.

There are instances where the intention is to model the dataset's probability density function rather than the data itself; for example, in generative models, the goal is to generate data similar to the dataset. To achieve this objective, variational models come into play, specifically Variational Auto-Encoders (VAE) [1]–[11] and Generative Adversarial Network (GAN) architectures [12]–[18]. The GAN architectures use a Generator and a Discriminator network and employ min-max training. During training, the generator network produces data samples of better quality at each time step to trick the discriminator, which learns to distinguish real data from fake data generated by the Generator network. In this manner, both networks engaged in min-max training learn to perform their respective tasks. The Generator produces more realistic data samples as the Discriminator becomes increasingly difficult to deceive. In terms of VAEs, these models approximate the dataset's probability density function by modeling its parameters [19] or by assigning an odds to each output [20], generating data from the random variable where each output holds the model's estimated odds. The resulting binary text classifier positioning of a dataset, this work posits that any problem for which the solutions can be encoded in an integer sequence can also be addressed in a generative manner. It is essential to assert that the optimization goal is expressible through a heuristic function, akin to the fitness function in the context of Genetic Algorithms (GAs) [21]–[30]. Heuristic search using Language Models suffers from a lack of exploration due to the well-known difficulty of stabilizing complex neural models when trained using Reinforcement Learning. Traditional issues include training convergence and subsequent hyperparameter tuning. Furthermore, RL is usually applied sequentially to causal problems. This paper proposes decoupling-based RL training techniques and network architecture design principles that enable the application of RL to new problem types, as well as the incorporation of Language Models' feature capture capabilities to address problems beyond linguistic ones. Considering the sequence encoding of the candidate solutions generated by the language model, an ontology must be defined to encode and serialize the candidates, allowing the architectures to generate data structures and refine them during training, similar to a GAN training setting. In contrast to traditional Heuristic Search methods, where the candidate solution can be an array of various degrees of freedom in the problem (e.g., variables in a multivariate optimization problem), language models can capture the data structure or ontology with the help of special characters. These characters are used in the sequence encoding, signaling the evaluation methodology to build and assess a diversity of data structures. This capability is referred to in this paper as Semantic Encoding. It is applied to the Neural Architecture Search downstream problem. The rest of this paper is organized as follows: II. Related Work, III. Semantic Encoding, IV. Proposed Architectures, V. Reinforcement Learning as a Search Methodology, VI. Decoupled Asynchronous Advantage Actor-Critic, VII. Decoupled Soft Q-Learning, VIII. Decoupling's Mathematical Formalization, IX. Proposed Training Formulation, X. Accessed Problems, XI. Results, XII. Error Analysis. Finally, the paper concludes with XIII. Conclusions and Future Work.

II. Related Work

The proposed heuristic search relates mainly to evolutionary algorithms, such as Genetic Algorithms. The adopted models are neural Language Models, and the training is based on Reinforcement Learning. In this section, all the aforementioned methods are detailed. Evolutionary algorithms can be seen as heuristic search engines in the sense that they generate candidate solutions, which are evaluated on the fly using a heuristic function, such as the fitness function in the case of Genetic Algorithms. Neural Language Models (LMs) are used for language modeling [31]–[38]. They learn meaningful features from text data through embedding generation techniques. When an LM is used in the context of Neural Machine Translation [36], [39]–[44], LMs can be viewed as generative models because they generate tokens that, when decoded, are words in the target language domain. This problem can be generalized into a Sequence2Sequence problem when considering the same language model architecture generating a sequence with a different semantic encoding than target language tokens, always restricted to a differentiable loss function. Neural Machine Translation (NMT) architectures are generative by nature because they produce tokens in the model's target language, although their training typically requires a differentiable loss function that might not accurately express the training goals. The same occurs in NAS tasks, where the primary objective is to increasingly enhance the candidate network's performance metric. In [45], a Recurrent Neural Network (RNN) is trained using Reinforcement Learning (RL) with the candidate network's performance almost directly serving as the reward function, employing various techniques to reduce the training's variance and facilitate learning through the described method. To relax the differentiable metric constraint, a new type of training is necessary; this is where Reinforcement Learning (RL) becomes relevant. RL techniques are primarily based on Markov Decision Processes (MDPs). Several training approaches attempt to optimize non-differentiable metrics in a deep model, such as surrogate losses [46], minimum risk training [47], and reinforcement learning [45]. All these training methodologies have their limitations: surrogate losses and reinforcement learning are difficult to stabilize, and minimum risk training is too computationally expensive when applied to a language model like an NMT architecture. Focusing on RL training, this article explores methods to stabilize the training and establish a robust optimization framework.

III. Semantic Encoding

Sequence semantic encoding is one of the core subjects in this proposal. When applied to the sequence generated by a Neural Machine Translation model, the problem can be transposed into an optimization problem where the candidates can be encoded as a sequence of integers [45]. The candidate solutions' meta-format can be a single value or a sequence of values, depending on the downstream problem. Special characters such as separators or sequence terminators can also be used to help specify the solution's evaluator behavior. The optimization problem structure that this kind of semantic encoding enables is a heuristic search, since the candidate solution's quality is evaluated by a reward function that can be non-differentiable, and its value can be generated during the search execution.

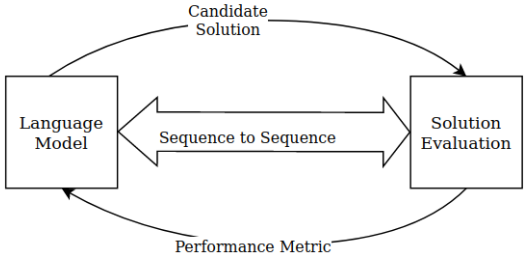

Figure 1. Heuristic search architecture.

For example, in order to access the Neural Architecture Search (NAS) problem using the proposed technique, the sequence can be the Network Structure Code (NSC), which encodes the candidate neural network hyperparameters. The network is then built and trained so that the performance metric can be extracted and the candidate sequence evaluated. Figure 1 highlights the proposed heuristic search architecture.

IV. Proposed Architectures

Depending on the nature of the problem, it can be beneficial to generate the sequence iteratively or through composition. As this article's subject is the usage of language models in optimization problems, and language models can encode semantics based on characters or words, both approaches will be explored further.

With the RL training enabled by the decoupling, based on unitary and semantically segmented tasks assigned to unitary model parts, the proposed architectures consist of two models inspired by character-level and word-level language models, respectively. With this training possibility, these models' generalization capability, as well as the proposed modeling principle, will be assessed.

A. Char-Conv with DeepQNet-Policy Learning

Starting from the model proposed in [48], two output kernels were used to decouple the tasks into position and value generation. In this way, one model pair, Q-Network and Policy-Net, is used to compose the candidate sequence. Regarding the Traveling Salesman Problem, a benchmark problem, the proposed training setting works without issues. When considering the Neural Architecture Search problem, the reward signal presents high variance and the training did not converge to zero. In addressing this problem, two changes were made: entropy regularization was added, and the output activation function was changed to linear so that the model output is interpreted as log probabilities for each output position.

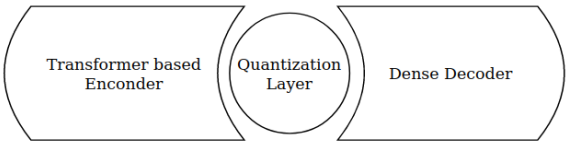

Figure 2. Vector Quantized Variational Auto-Encoder proposed architecture. The encoder comes from the Transformer architecture, the quantization layer from [20], and the decoder is made of stacked dense layers.

B. Transformer-based Vector Quantized Variational Auto-Encoder with Asynchronous Advantage Actor Critic

The word-level model is based on the Transformer architecture proposed in [49], which includes both the Transformer encoder and decoder architectures, along with the vector quantization layer proposed in [20]. This Vector Quantized Variational Autoencoder (VQ-VAE) architecture was decoupled as well; however, in this case, its outputs correspond to the actor and the critic. The actor outputs log probabilities for the possible actions of the RL agent, and the critic rates the inputs. Maintaining the sequence composition decoupling strategy, two models are employed to compose the target sequence. Once again, one model specializes in generating the position, while the second model generates the value to be assigned. Figure 2 illustrates the architecture utilized for the VQ-VAE.

V. Reinforcement Learning as a Search Methodology

Since the search for optimal solutions is guided by reinforcement learning, the model generates multiple candidate solutions and iteratively improves them based on feedback. A heuristic evaluation function $g : \mathcal{Y} \to \mathbb{R}$ assigns a quality score to candidate solutions, serving as a reward signal:

$$R(y) = g(y). \tag{1}$$

Given any problem where the solution space $\mathcal{Y}$ is structured as integer sequences, the proposed methodology guarantees:

- **Expressibility**: The model $\hat{f}_\theta$ can learn to generate valid sequences from $\mathcal{X}$ using neural networks that are trained on $\mathcal{D}$.
- **Optimization Capability**: The reinforcement learning-based search ensures that generated solutions are iteratively improved using $g(y)$.
- **Generalization**: The auto-regressive nature of the model allows it to generate variable-length solutions applicable to different instances of the problem since a special character can be used as a sequence terminator.

Thus, for any integer-encoded problem, the formulation is sufficient to obtain high-quality solutions through iterative refinement. The proposed formulation applies to a wide range of problems where solutions are represented as integer sequences, including:

- Combinatorial optimization problems (e.g., the Traveling Salesman Problem, Knapsack Problem).
- Scheduling and planning tasks where actions are encoded as integer sequences.
- Code synthesis and symbolic regression.
- Game strategies with discrete action spaces.
- Non-sequential problems that benefit from value-position decoupling.

For any such problem, the integer-encoded representation ensures that the model can map problem instances to structured sequences and refine them over iterations using reinforcement learning. The search methodology follows a reinforcement learning-based approach such as DQN-PL [50], [51], A3C [52], and SoftQ-Learning [53]. The exploration methodology is epsilon-greedy for all the approaches. The different training methodologies are described in the next subsections.

VI. Decoupled Asynchronous Advantage Actor Critic

The main concept in decoupling is to create a problem feature extraction core and decoupled output decoders to model the output value according to the problem's required output. For example, in the VQ-VAE with the A3C training case, the same model generates the action and its corresponding critic value. To generate a sequence, two models with the specified decoupling are used: one generates the position of the new element, and the second generates its value. The resulting sequence is then updated and iteratively refined. Next, the formal formulation of this kind of decoupling is provided.

A. Policy and Value Functions

Let S be the state space, A be the action space, and $P(s'|s, a)$ be the transition probability. The reward function is defined as $R(s, a, p)$, where p is the selected position.

The policy consists of two independent components:

$$\pi(a|s; \theta_a) \quad \text{and} \quad \pi(p|s; \theta_p) \tag{2}$$

where:

- $\pi(a|s; \theta_a)$ selects an action based on state s.
- $\pi(p|s; \theta_p)$ selects a position based on state s.

The value functions are defined as:

$$V_{\text{act}}(s; \theta_v) = \mathbb{E}\left[R(s, a, p) + \gamma V_{\text{act}}(s')\right] \tag{3}$$

$$V_{\text{pos}}(s; \theta_p) = \mathbb{E}\left[R(s, a, p) + \gamma V_{\text{pos}}(s')\right] \tag{4}$$

B. Exploration-Exploitation Strategy

The exploration rate for both action and position selection follows an epsilon-greedy decay:

$$\epsilon_a(t + 1) = \max(\epsilon_a(t) \cdot d, \epsilon_{\min}) \tag{5}$$

$$\epsilon_p(t) = \epsilon_a(t) \tag{6}$$

where d is the decay factor and $\epsilon_{\min}$ is the minimum exploration rate.

C. Advantage Function and Returns

The advantage function for actions is given by:

$$A_{\text{act}}(s,a) = r + \gamma V_{\text{act}}(s') - V_{\text{act}}(s) \tag{7}$$

The advantage function for positions is:

$$A_{\text{pos}}(s,p) = r + \gamma V_{\text{pos}}(s') - V_{\text{pos}}(s) \tag{8}$$

The discounted return at timestep t is:

$$G_t = \sum_{k=0}^{T-t} \gamma^k R(s_{t+k}, a_{t+k}, p_{t+k}) \tag{9}$$

The returns are then normalized:

$$\hat{G_t} = \frac{G_t - \mu(G)}{\sigma(G) + \epsilon} \tag{10}$$

D. Loss Functions

The critic losses for action and position value networks are:

$$L_{\text{critic-act}} = \sum_t \left(A_{\text{act}}(s_t, a_t)\right)^2 \tag{11}$$

$$L_{\text{critic-pos}} = \sum_t \left(A_{\text{pos}}(s_t, p_t)\right)^2 \tag{12}$$

The actor losses are:

$$L_{\text{actor-act}} = -\sum_t \log \pi(a_t|s_t) A_{\text{act}}(s_t, a_t) \tag{13}$$

$$L_{\text{actor-pos}} = -\sum_t \log \pi(p_t|s_t) A_{\text{pos}}(s_t, p_t) \tag{14}$$

The total losses are:

$$L_{\text{total-act}} = L_{\text{actor-act}} + L_{\text{critic-act}} \tag{15}$$

$$L_{\text{total-pos}} = L_{\text{actor-pos}} + L_{\text{critic-pos}} \tag{16}$$

E. Gradient Updates

Gradients for action and position networks are computed separately:

$$\nabla_{\theta_a} L_{\text{total-act}} = \sum_t \nabla_{\theta_a} L_{\text{total-act}} \tag{17}$$

$$\nabla_{\theta_p} L_{\text{total-pos}} = \sum_t \nabla_{\theta_p} L_{\text{total-pos}} \tag{18}$$

These gradients are applied using an optimizer:

$$\theta_a \leftarrow \theta_a - \alpha \nabla_{\theta_a} L_{\text{total-act}} \tag{19}$$

$$\theta_p \leftarrow \theta_p - \alpha \nabla_{\theta_p} L_{\text{total-pos}} \tag{20}$$

where α is the learning rate.

This content was generated with the help of generative artificial intelligence [54].

VII. Decoupled SoftQ-Learning

Regarding the CharConv model in the NAS problem assessment, it was not possible to stabilize the training using the traditional DQN-PL approach. In the NAS setting, it was found beneficial for training stability to use stochastic outputs followed by a random experiment with the model's predicted output odds to generate the predicted action. To help stabilize the training in a stochastic environment, entropy regularization was employed.

Concerning the decoupling technique used in this context, two models were utilized. One model features a CharConv core and two decoupled outputs: one for value and another for the position of the new element in sequence generation. The second model is the target network, which generates the stochastic SoftQ-values for each output.

Additionally, an epsilon-greedy exploration strategy was applied in conjunction with an experience replay buffer. The proposed SoftQ-Learning approach uses a different decoupling when compared to the method presented in the previous section. This is specified in the subsequent subsections.

A. State and Action Representation

Let $s \in \mathcal{S}$ be the state space and $a \in \mathcal{A}$ be the action space. Additionally, let $p \in \mathcal{P}$ denote the position selection space. The agent selects both an action and a position at each time step.

B. Soft Q-Function

Define the Q-function as:

$$Q(s,a,p) = Q_{\text{action}}(s,a) + Q_{\text{position}}(s,p). \tag{21}$$

This decoupling allows independent learning of action and position values.

C. Soft Q-Learning Update Rule

The update rule follows the soft Bellman equation:

$$Q_{\text{action}}(s,a) \leftarrow (1-\alpha) Q_{\text{action}}(s,a) + \alpha \left[r + \gamma \tau \log \sum_{a'} \exp\left(\frac{Q_{\text{action}}(s',a')}{\tau} \right) \right], \tag{22}$$

$$Q_{\text{position}}(s,p) \leftarrow (1-\alpha) Q_{\text{position}}(s,p) + \alpha \left[r + \gamma \tau \log \sum_{p'} \exp\left(\frac{Q_{\text{position}}(s',p')}{\tau} \right) \right]. \tag{23}$$

where:

- α is the learning rate,
- γ is the discount factor,
- τ is the temperature parameter for soft Q-learning,
- r is the received reward,
- s' is the next state.

D. Action and Position Selection

The action and position are selected using the softmax policy:

$$P(a|s) = \frac{\exp(Q_{\text{action}}(s,a)/\tau)}{\sum_{a'} \exp(Q_{\text{action}}(s,a')/\tau)}, \tag{24}$$

$$P(p|s) = \frac{\exp(Q_{\text{position}}(s,p)/\tau)}{\sum_{p'} \exp(Q_{\text{position}}(s,p')/\tau)}. \tag{25}$$

This formulation [55] allows efficient and structured learning by decoupling position and value, improving performance in reinforcement learning tasks that require both action selection and spatial positioning.

In the next section the position-value decoupling for integer-based sequences is formalized.

VIII. Decoupling's Mathematical Formalization

When considering an iteratively generated sequence, in which the elements are generated one after another, the position is fixed and incremental, which implies causality in the sequence generation. By decoupling the functionality into position generation and value generation, thereby composing a single sequence (RL state), it is possible to break the causality implication and still utilize the reinforcement learning capability of optimizing heuristic functions. In this article, the decoupling is achieved at an architectural level; in a multi-branch architecture, each output branch is responsible for one single decoupled task in the non-causal sequence generation. To optimize a single sequence using two models, the state must be shared, and the RL techniques must still be applied to each model, utilizing separate optimizers guided by the same resulting reward.

In incremental sequence generation, this type of sequence generation allows for imposing causality in the RL agent's behavior, leading to a succession of actions generated throughout the training. Regarding compositional sequence generation, where the problem focus is to generate a candidate answer encoded in the sequence rather than a set of actions, decoupling can come into play to divide and conquer the generation problem into two sub-problems, enabling the composition of the sequence without needing to condition on the previous actions.

To extend RL beyond causal MDPs, we decompose the Q-function as follows:

$$Q(s,a) = P(s) + A(s,a), \tag{26}$$

where:

- $P(s) = \mathbb{E}[R|s]$ is the **position value**, which captures the expected reward at state s independent of actions.
- $A(s,a) = Q(s,a) - P(s)$ is the **advantage function**, representing the additional benefit of taking action a beyond merely being in state s.

If actions have no influence (a fully non-causal setting), then $A(s,a) = 0$, reducing RL to pure statistical inference:

$$V(s) = P(s) = \mathbb{E}[R|s]. \tag{27}$$

The objective function is defined as:

$$J(\pi) = \mathbb{E}_{s\sim D}[P(s)], \tag{28}$$

where D is a dataset of observed states and rewards. If actions have partial influence, it is optimized as follows:

$$J(\pi) = \mathbb{E}_{s,a\sim D}[P(s) + A(s,a)]. \tag{29}$$

This formulation bridges RL and supervised learning, enabling RL in non-causal settings, such as:

- Counterfactual reasoning.
- Offline and batch RL.
- Decision-making in complex, non-Markovian environments.

IX. Proposed Training Formulation

In this section, two training algorithms for Heuristic Optimization are proposed: the VQ-VAE model with A3C training and Char-Conv with DQNet-PL, so both character-level and word-level language models are explored.

We define the problem as a Markov Decision Process (MDP) with:

- State space: S
- Action space: A
- Transition dynamics: P
- Reward function: R

The objective is to learn a policy π that maximizes the cumulative expected reward.

A. State Representation

The state at time t, denoted as s_t, represents the environment state:

$$s_t \in S. \tag{30}$$

B. Action Selection

A neural network models the probability distribution for action selection:

$$a_t \sim \pi(a_t|s_t;\theta). \tag{31}$$

The chosen action a_t is sampled from this distribution.

C. Critic Network (Value Estimation)

A critic network estimates the value function $V(s_t)$, representing the expected return from state s_t:

$$V(s_t) = \mathbb{E}\left[\sum_{k=0}^{\infty} \gamma^k r_{t+k}\right]. \tag{32}$$

D. Reward and Return Calculation

The immediate reward r_t is received from the environment. The discounted return is computed as:

$$G_t = r_t + \gamma G_{t+1}. \tag{33}$$

The returns are then normalized:

$$\hat{G_t} = \frac{G_t - \mu}{\sigma + \epsilon}. \tag{34}$$

E. Advantage Estimation

The advantage function measures how much better the taken action was compared to the expected return:

$$A_t = \hat{G}_t - V(s_t). \tag{35}$$

F. Actor-Critic Loss Functions

The loss for the actor (policy gradient) is:

$$L_{\text{actor}} = -\sum_t \log \pi(a_t|s_t) A_t. \tag{36}$$

The critic is updated using the Huber loss:

$$L_{\text{critic}} = \sum_t \text{Huber}(V(s_t), \hat{G}_t). \tag{37}$$

The Huber loss is defined as:

$$\text{Huber}(x, y) = \begin{cases} \frac{1}{2}(x-y)^2, & \text{if } |x-y| < \delta \\ \delta(|x-y| - \frac{1}{2}\delta), & \text{otherwise} \end{cases} \tag{38}$$

G. Gradient Update

The gradients of the total loss function are computed as:

$$\nabla_\theta L_{\text{total}} = \nabla_\theta (L_{\text{actor}} + L_{\text{critic}}). \tag{39}$$

The parameters are updated using the Adam optimizer:

$$\theta \leftarrow \theta - \alpha \nabla_\theta L_{\text{total}}. \tag{40}$$

H. Termination Criteria

Training stops when the running reward exceeds a threshold:

$$\sum_t r_t > R_{\text{target}}. \tag{41}$$

This indicates that the agent has effectively learned an optimal policy for the given task. In this A3C setting, two models are used in order to generate the sequence. In each step a new value and its corresponding position in the sequence (RL state) are generated. Each model has two outputs: one for the action and another for the critic score.

I. Char Conv + DQN-PL

1. Q-Function Approximation

We approximate the action-value function (Q-function) by a neural network with parameters θ:

$$Q(s, a; \theta) \approx \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t r_t \,\middle|\, s_0 = s, a_0 = a\right],$$

where:

- s is the state,
- a is the action,
- r_t is the reward at time t,
- γ is the discount factor.

2. Experience Replay

Experiences are stored in a replay buffer as tuples:

$$(s, a, r, s', d),$$

where d is an indicator that equals 1 if s' is terminal and 0 otherwise.

A mini-batch of N experiences is sampled uniformly at random from the replay buffer for training.

3. Target Calculation

For each sampled experience (s, a, r, s', d), the target value y is computed as:

$$y = r + \gamma \max_{a'} Q(s', a'; \theta^-) \cdot (1 - d),$$

where θ^- denotes the parameters of the target network, which are periodically updated to match the primary network parameters θ.

4. Loss Function

The loss function for a mini-batch is defined as the mean squared error between the target and the current Q-value estimate:

$$L(\theta) = \frac{1}{N} \sum_{i=1}^{N} \left(y_i - Q(s_i, a_i; \theta)\right)^2.$$

This loss is minimized to update the parameters θ of the Q-network.

5. Gradient Descent Update

The parameters θ are updated via gradient descent:

$$\theta \leftarrow \theta - \alpha \nabla_\theta L(\theta),$$

where α is the learning rate.

6. Action Selection (Epsilon-Greedy Policy)

At each step, the action a is chosen according to the epsilon-greedy strategy:

$$a = \begin{cases} \text{random action}, & \text{with probability } \epsilon, \\ \arg\max_{a'} Q(s, a'; \theta), & \text{with probability } 1 - \epsilon, \end{cases}$$

with ϵ decaying over episodes from an initial value ϵ_{start} to a minimum value ϵ_{min}.

7. Periodic Target Network Update

Every fixed number of episodes (or steps), the target network parameters are updated by copying the weights from the primary network:

$$\theta^- \leftarrow \theta$$

X. Accessed Problems

For each of the two described ways to generate sequences, causal or non-causal, and regarding the Reinforcement Learning (RL) usage along with the proposed architectures, one benchmark problem was selected. The Traveling Salesman Problem (TSP) for causal generation and Neural Architecture Search (NAS) for non-causal generation.

A. Traveling Salesman Problem

The TSP consists of generating a tour from a given starting city that passes through all the other cities while minimizing the overall path distance. The considered cities have the following coordinates:

TABLE I. CITIES' COORDINATES USED IN THE TRAVELING SALESMAN PROBLEM.

X	Y
23	45
57	12
38	78
92	34
45	67
18	90
72	55
66	24
83	62
49	40

A distance matrix is calculated based on the euclidean distance between all the cities. A boolean array is used to track the cities already visited. If a generated city is already visited, the reward function gets the value of -100, in contrary, if a city is not visited, then the reward function gets the value given by:

$$\text{normalized\_reward} = 100 \cdot \left(1 - \frac{\text{distance}}{\text{max\_distance}}\right)$$

With:

$$\text{distance} = \text{distance\_matrix}[\text{current\_city}][\text{action}]$$

The cities road is generated iteratively, one city after another until the generated city is already visited. When this final condition is met, the obtained road is evaluated and the current episode ends.

B. Neural Architecture Search

For the NAS problem, the sequence is interpreted as the Network Structure Code (NSC), meaning that it encodes an Artificial Neural Network (ANN). In this case, it is intended to generate a neural text classifier architecture built by several InceptionV1 blocks [56]. The NSC is composed by two decoupled models which contribute to the same RL final state, also known as NSC. The reward function is the child-network training accuracy which, in the current problem's case, is a classifier network. This classifier is built from an inverted n-ary tree encoded in Depth-First-Search (DFS).

XI. RESULTS

In this section, the performance plots for the NAS problem are presented. The adopted search space is an encoded n-ary tree using Depth First Search (DFS). The tree is encoded using $[0, 1, 2]$ in a sequence with a maximum of five positions. A zero encodes a change in the tree branch, a one encodes a deeper instruction, and the two is interpreted as a padding character. Each tree element is a Conv1D version of an InceptionV1 block [56]. When constructed, the tree is inverted so that the root node represents the classifier's final decision kernel. The search focuses on a text classifier, where the embeddings are provided by a Keras embedding layer. For evaluation purposes, this layer is replaced by the RoBERTa large model from Hugging Face [57], achieving state-of-the-art results with the IMDB sentiment analysis dataset [58]. The resulting model from the search was trained using a learning rate scheduler and presents the training curves shown in Figure 3.

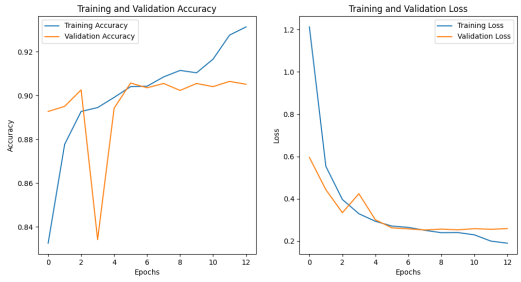

Figure 3. Classification accuracy and binary cross-entropy loss when using the generated NAS classifier and RoBERTa as embedding model.

The resulting binary text classifier positioning in the state of the art is presented in Table III.

TABLE II. FINAL MODEL RESULTS ON IMDB SENTIMENT ANALYSIS DATASET.

Test Loss	0.2521449327468872
Test Accuracy	0.9054897427558899

The results presented were obtained by replacing the embedding layer with a pre-trained model from [59].

TABLE III. IMDB SENTIMENT ANALYSIS TEST SET ACCURACY FOR DIFFERENT MODELS IN THE LITERATURE

Model	Accuracy (%)	Reference
Naive Bayes (Baseline)	83.5	[60]
LSTM (Long Short-Term Memory)	89.0	[61]
BiLSTM with Attention	91.2	[62]
FastText	88.5	[63]
RoBERTa+NAS Tree-based Classifier	90.5	-
CNN (Convolutional Networks)	90.6	[64]
ULMFiT (Pretrained LSTM)	94.0	[65]
BERT-base (Fine-tuned)	95.2	[66]
RoBERTa (Fine-tuned)	96.3	[67]
DistilBERT	95.1	[68]
GPT-2 (Fine-tuned)	95.0	[69]
XLNet	96.4	[70]
ALBERT	95.8	[71]
ELECTRA	96.6	[72]
T5 (Text-to-Text Transfer)	96.1	[73]
GPT-3 (Few-shot)	94.7	[74]
DeBERTa (Fine-tuned)	96.7	[75]
ChatGPT (Prompting)	96.0*	[76]

The neural architecture search task was performed using both language models: character-level using SoftQLearning

and word-level using asynchronous advantage actor-critic training. In both cases, the problem's probability density function for each output was predicted by the models, and the final output is a result of a random experience with the model-predicted odds. This feature allows the models to represent more complex problems, such as NAS. This behavior also enables the model to learn the probabilistic aspects of a dataset; by fixing a serializable data ontology, it can generate datasets. Returning to the scope of this article, more specifically regarding these models' optimization capability in the NAS task, the learning and performance curves are presented below.

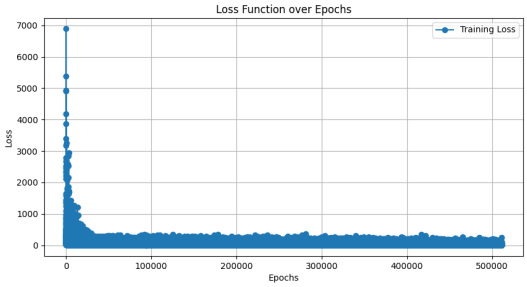

Figure 4. Loss function of SoftQ-Leaning using Char-Conv inspired architecture.

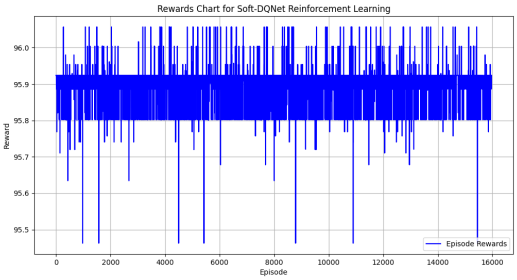

Figure 5. RL reward function, child network's training accuracy, using SoftQ-Leaning using Char-Conv inspired architecture.

In the above experiment the model presented in [48], has two decoupled outputs which are used to compose the sequence - Network Structure Code. The Soft Q-Learning training method was adopted instead of DQNet-PL because the latest presents a very high training variance, making the training to not converge. Additionally the entropy regularization also helped to attain training convergence.

The transformer-based Vector Quantized Variational Auto Encoder (VQ-VAE) follows the same decoupling logic to compose the sequence, as described previously. In this case, the model has two outputs: the actor and the critic. The actor predicts odds for each possible model action, and the second output, the critic rates the overall model performance. In terms of architecture, the actor-critic decoupling is made only in the model's last layer to shape the output according to the needs to generate the critic score and actor's odds.

Two Transformer-based VQ-VAE models were used to compose the sequence, one to generate the action and another to generate the position in the candidate sequence where the action value will be assigned. Bellow, the obtained training curves are presented:

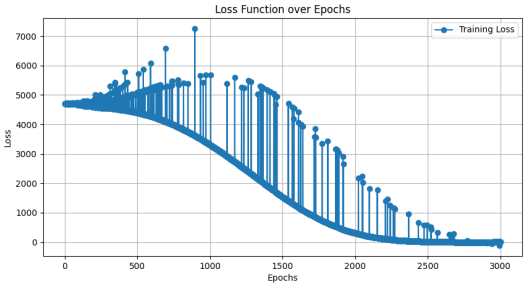

Figure 6. Loss function of action sequence composing parameter during the A3C training using Transformer inspired architecture.

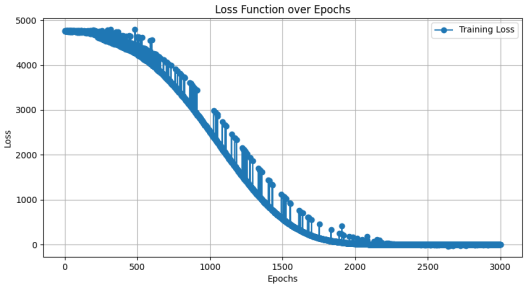

Figure 7. Position loss function of A3C using Transformer inspired architecture.

The observable outliers are due to the epsilon-greedy technique used to introduce exploration in the algorithm's behavior. All the loss function plots in the presented results converge to zero, and the reward signals reflect the overfitting tendency of the proposed NAS methodology. The decoupling strategies are effective in stabilizing the training methodologies in both character and word-level approaches. Additionally, the sequence generalization and problem modeling capabilities are

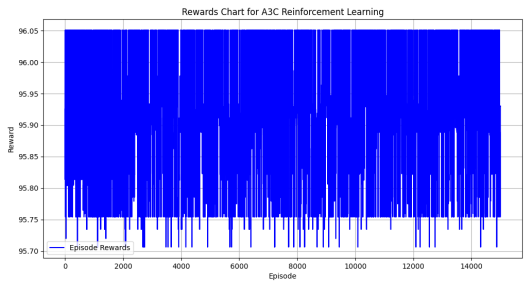

Figure 8. RL reward and child network accuracy as functions of A3C using a Transformer-inspired architecture.

verified when observing the obtained training curves; both approaches exhibit stable behavior.

Next, the Traveling Salesman Problem results are presented. Experiments with both the architectures are presented bellow.

Starting from the Char-Conv as DQNet and as well as Policy network, the results were the following:

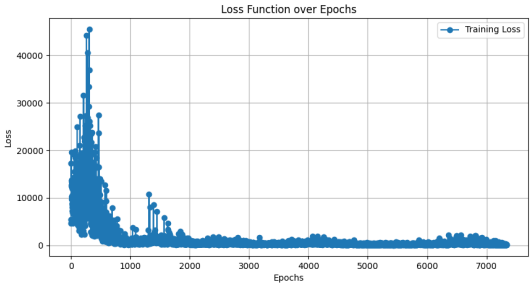

Figure 9. Char-Conv architecture's loss function during the DQNet-PL training, while solving the Traveling Salesman problem.

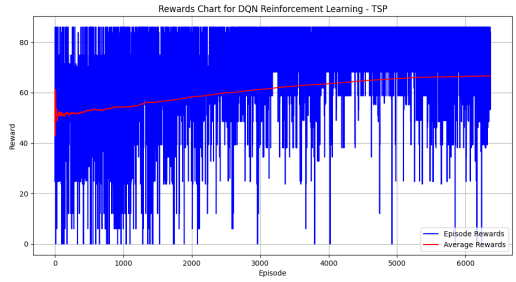

Figure 10. Reward function of Char-Conv architecture during the DQNet-PL training, while solving the TSP problem.

Both curves indicate that the RL agent is learning, as evidenced by the loss function's convergence to zero and the reward function's increasing behavior during training. Next, the VQ-VAE model is used in conjunction with A3C training to generate the salesman route:

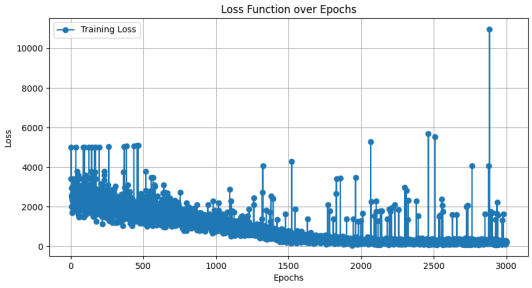

Figure 11. Loss function during the A3C training using Transformer inspired architecture in the TSP problem resolution.

The loss function chart exhibits zero convergence; therefore, training stability is concluded, and the generally increasing reward function reflects the VQ-VAE agent's learning. Depending on the problem complexity, generating action odds might

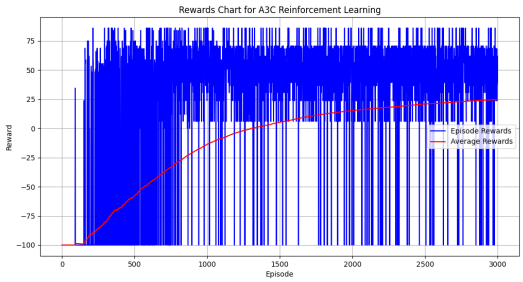

Figure 12. Reward function obtained by the VQ-VAE based agent in A3C.

be preferred rather than generating the agent's actions directly, as occurred with the Char-Conv architecture in NAS, where Soft-Q Learning was used, and in the TSP where DQNet-PL was utilized. The Transformer-inspired VQ-VAE demonstrates overall better training behavior compared to the Char-Conv architecture, as this model can map the search space into several sub-regions by utilizing the Vector-Quantized layer, thereby parallelizing the search.

XII. Error Analysis

During the experimentation phase of this work, the Traveling Salesman benchmark problem was addressed using A3C training together with the Transformer-based VQ-VAE model. Additionally, the Char-Conv model was tested alongside DQNet-PL training on the same problem. After several unsuccessful experiments resulted from the usual issues of high variance in the reward signal and a non-converging loss function, a functional decoupling methodology was developed and successfully applied to the TSP problem. The training results are presented in Figures 9 and 11 for the Char-Conv and VQ-VAE models, respectively.

In considering the NAS problem, the combination of Char-Conv with DQN-PL training did not succeed in solving this issue, as the loss function did not converge to zero. In contrast, the combination of VQ-VAE, A3C, and the respective decoupling effectively solved the problem (Figures 6 and 7). To address the limitations of solving the NAS problem using CharConv, SoftQ Learning with entropy regulation was employed, as it enables modeling the odds of each output and reduces the variance of the reward signal.

XIII. Conclusions and Future Work

Many problems are non-sequential and do not require strict left-to-right order dependency. To handle such cases, a value-position decoupling strategy is proposed. Considering the Transformer-based VQ-VAE trained with A3C, the model has two outputs: an actor output and a critic output. Instead of using two models, a single model is employed. In this way, the network weights are updated on both occasions: when the actor learns and when the critic learns. Two A3C models with a shared state and reward are used; one generates the new element's position, and the other generates the new element's values. The VQ-VAE architecture has the capability

to divide the latent space into quantized subspaces and perform a parallelized search in each subspace.

The deep convolutional network, which is trained using Deep Q-Learning for value generation and Soft Q-Learning for sequence generation, applies similar reasoning to design the training. One model with two outputs is responsible for generating the new element's position, while another model generates the new element's value. To make this training generative, the output odds are modeled, and the outputs are generated using a random experiment in which each output odd is defined by the Deep Q-models. Additionally, to reduce training variance, an entropy term is added to the loss function. This process is called entropy regularization and promotes training convergence towards zero.

This study demonstrates that it is possible to generate sequences without causality constraints while still using slightly adapted Reinforcement Learning techniques. Training convergence is improved if the same model with two outputs is used to perform actions and to critique its performance, regardless of its architecture. In both cases, Transformer and Char-Conv, it was the most performant architectural variation and performed heuristic search in this manner. Complex ontologies describing the candidate solutions can be encoded and serialized into integer sequences. The encoded sequences can then be optimized by this type of solver when used together with a performance metric designed as the Reinforcement Learning reward. Since sufficient decoupling is achieved, the language models can absorb the problem's semantics and generate admissible candidate solutions of increasing quality. The position-value decoupling must be employed in the NAS scenario to avoid imposing causality in the sequence generation during the RL training. Additionally, using variational models in complex RL environments such as NAS is more efficient since they model the environment's unknown properties. The Transformer-based VQ-VAE is also capable of parallelizing the search due to the vector quantization layer.

Looking toward the future, the models presented, along with the proposed training techniques, can be used to generate more than encoded solutions for a given problem. By selecting an appropriate reward function, the generated sequence can be utilized in the standard format to produce content, similar to Generative Adversarial Networks.

A comparison of the proposed solvers, together with other state-of-the-art heuristic search algorithms, can be made to systematically explore the limitations of this proposal and extend its applicability domain. An analysis of the problem's degrees of freedom versus processing time will be conducted, focusing on solver quality analysis based on degrees of freedom, the solver's scaling with DoF, and the algorithm's parallelization.

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