Non-Emptiness for UHATs Is $\mathrm{EXPSPACE}$-Hard

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Problem Statement & Proof Roadmap

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Problem (Non-Emptiness for UHAT)

Given a UHAT T, decide if $L(T) \neq \emptyset$.

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Why is this interesting?

Non-emptiness is a minimal verification question. If even this is EXPSPACE-hard, then richer verification tasks such as equivalence, universality, or property checking should not be expected to be easy in full generality.

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Today we show one of the main results by Bergstraßer et al.[1]:

Theorem

The non-emptiness problem for UHAT is EXPSPACE-hard.

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Proof Roadmap

Theorem (2^n-tiling)

2^n-tiling problem (will be introduced) is EXPSPACE*-complete*[2].

[2] F. Schwarzentruber, "The Complexity of Tiling Problems," arXiv:1907.00102, 2019.

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Lemma (2^n-tiling $\rightarrow$ B-RASP programs)

2^n-tilling problems are polynomial time reducible to the non-emptiness problems for B-RASP programs.

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Lemma (B-RASP programs $\rightarrow$ UHATs)

Non-emptiness problems for UHATs are polynomial time reducible to the non-emptiness problems for B-RASP programs.

Theorem (A Lower Bound)

The non-emptiness problem for UHAT is $\mathrm{EXPSPACE}$*-hard.*

$$2^n\text{-Tiling} \leq_p \text{B-RASP Non-Emptiness} \leq_p \text{UHAT Non-Emptiness}$$

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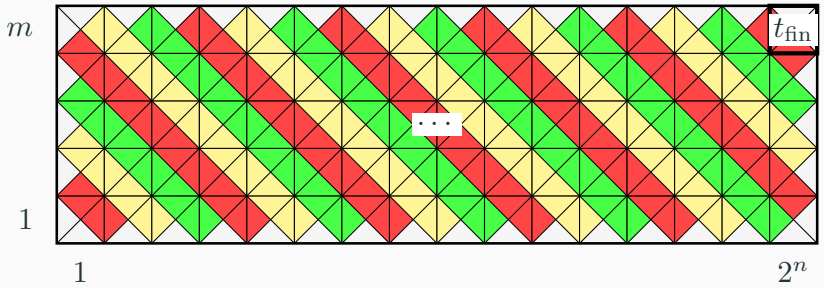
2^n-tiling Problem (EXPSPACE-complete!)

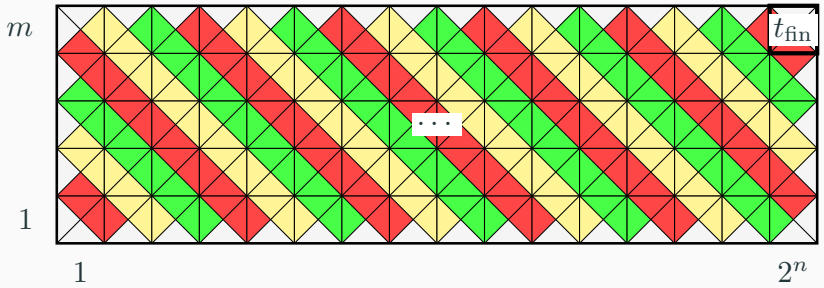


Definition (Tiles)

A *tile* is a quadruple $t \in \mathbb{N}_0^4$, where we write

$$t = \langle \text{left}(t), \text{up}(t), \text{right}(t), \text{down}(t) \rangle.$$

2^n-tiling Problem (EXPSPACE-complete!)



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Given (1) An integer $n > 0$ in unary, (2) a finite set T of tiles, and (3) a tile $t_{fin} \in T$,

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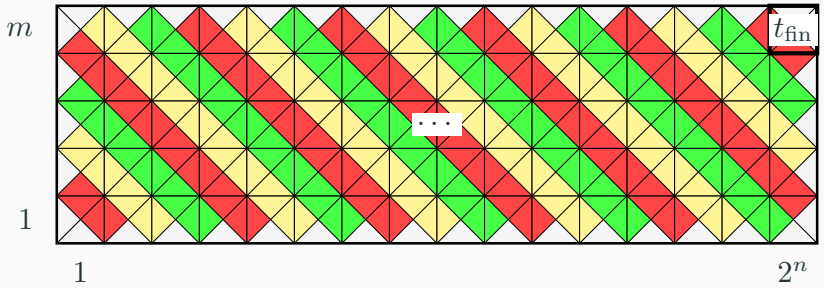

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Given (1) An integer $n > 0$ in unary, (2) a finite set T of tiles, and (3) a tile $t_{fin} \in T$, does there exist an interger $m > 0$ and a function $\tau : \{1, \ldots, 2^n\} \times \{1, \ldots, m\} \to T$

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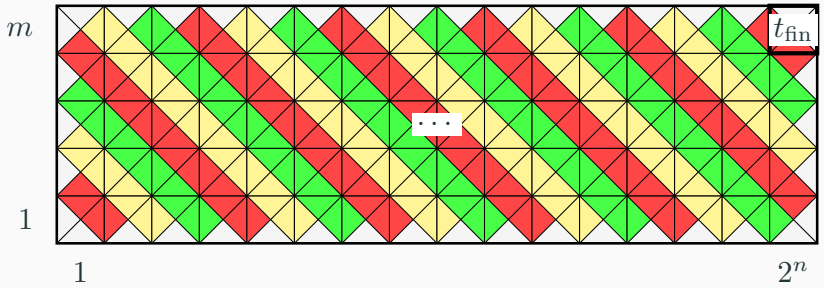

Problem (2^n-tiling)

Given (1) An integer $n > 0$ in unary, (2) a finite set T of tiles, and (3) a tile $t_{fin} \in T$, does there exist an interger $m > 0$ and a function $\tau : \{1, \ldots, 2^n\} \times \{1, \ldots, m\} \to T$ such that (1) $\tau(2^n, m) = t_{fin}$, (2) $\mathrm{down}(\tau(i, 1)) = \mathrm{up}(\tau(i, m)) = 0$ for all $1 \leq i \leq 2^n$, (3) $\mathrm{left}(\tau(1, j)) = \mathrm{right}(\tau(2^n, j)) = 0$ for all $1 \leq j \leq m$, (4) $\mathrm{right}(\tau(i, j)) = \mathrm{left}(\tau(i + 1, j))$ for all $1 \leq i < 2^n$ and $1 \leq j \leq m$, and (5) $\mathrm{up}(\tau(i, j)) = \mathrm{down}(\tau(i, j + 1))$ for all $1 \leq i \leq 2^n$ and $1 \leq j < m$.

2^n-tiling $\leq_p$ B-RASP non-emptiness

Recap on B-RASP programs

Vectors P_i in Restricted Access Sequence Processing (RASP)

- A feature vector assigns one value to each position of the input.
- A Boolean vector can record whether some property is true at each position.
- $Q_a(i) = 1 \Leftrightarrow w(i) = a$.

	1	2	3	4	5
input w	a	b	b	a	c
$P_1(Q_a)$	1	0	0	1	0
$P_2(Q_b)$	0	1	1	0	0
$P_3(Q_c)$	0	0	0	0	1
P_4	0	1	0	0	0

P_4: position i is the first b.

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Definition (Sketching B-RASP)

- A *B-RASP* program *builds* new features with basic token features $(Q_a, Q_b, \dots)$.
- One of the vectors is designated as the *output vector* deciding acceptance.

	1	2	3	4	5
input w	a	b	b	a	c
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P_4	0	1	0	0	0

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Recap on B-RASP programs: Building Operations

Position-wise operation

$P_{t+1}(i) := R(i)$, where $R(i)$ is some Boolean combination of $\{P_1(i), \ldots, P_t(i)\}$.

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Attention operation

An attention operation defines a new feature vector P_{t+1} by letting each position i look at one selected position j,

$$P_{t+1}(i) := \triangleright_j [M(i,j), S(i,j)]\, V(i,j) : D(i),$$

where S, V, D are Boolean combinations of $\{P_1(i), \ldots, P_t(i)\}$.

- $M(i,j)$ is the mask, saying which positions j are visible from i.
- $S(i,j)$ is the score predicate, saying which visible positions are relevant.
- $\triangleright_j$ means: choose the rightmost visible j such that $S(i,j) = 1$.
- If such a position j exists, set $P_{t+1}(i) := V(i,j)$. If no such position exists, use the default value: $P_{t+1}(i) := D(i)$.

2^n-tiling $\leq_p$ B-RASP non-emptiness: Encoding τ as a word

We encode a configuration of tiles (τ) as a word over the alphabet $\Sigma := T \cup \{0, 1, \#\}$.

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Encoding Scheme

1. Define $\mathrm{enc}_\tau : \{1, \ldots, 2^n\} \times \{1, \ldots, m\} \to \Sigma^*$ by $\mathrm{enc}_\tau(i, j) := \langle i - 1 \rangle \tau(i, j) \#$ for all $i \in [1, 2^n]$ and $j \in [1, m]$, where $\langle i - 1 \rangle$ denotes the binary encoding of $i - 1$.

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2. Define $\mathrm{enc}(\tau) := \mathrm{enc}_\tau(1, 1) \cdots \mathrm{enc}_\tau(2^n, 1) \mathrm{enc}_\tau(1, 2) \cdots \mathrm{enc}_\tau(2^n, m)$.

Example

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We construct a B-RASP program that accepts $\mathrm{enc}(\tau)$ iff τ satisfies the conditions.

The construction: form checking

Example

$0000a_1\#0001a_2\#0010a_3\#\cdots\#1111a_{2^4}\#$. ($n = 4$, $m = 1$ and $a_i \in T$ for $i \in [2^4]$.)

We first check if the input is of the form $(\{0,1\}^n T\#)^*$ by the following vectors.

$$A_T(i) := \blacktriangleright_j\, [j < i, 1] \bigvee_{t \in T} Q_t(j) : 0$$

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$$A_{enc}(i) := (Q_\#(i) \to A_T(i)) \wedge \left(\left(\bigvee_{t\in T} Q_t(i)\right) \to \left(\bigwedge_{k=1}^{n} A_{C,k}(i)\right) \wedge A_{\#,n+1}(i)\right)$$

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A(i) &:= \blacktriangleright_j\, [j < i, \neg A_{enc}(j)]\, 0 : A_{enc}(i).
\end{aligned}
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$$A(i) :=\blacktriangleright_j\ [j < i, \neg A_{enc}(j)]\, 0 : A_{enc}(i).$$

Require $A(|enc(\tau)|) = 1$.

The construction: counter checking

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$$C_1(i) :=\blacktriangleright_j\ [j < i, Q_0(j) \vee Q_1(j)]Q_1(j) : 0$$

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$$\left(\bigwedge_{r=k+1}^{n} C_r(i) \leftrightarrow C_r(j) \right) : 0$$

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$$C_{1\to 0}(i) :=\blacktriangleright_j\ [j < i, Q_\#(j)] \bigwedge_{k=1}^{n} \neg C_k(i) \wedge C_k(j) : \bigwedge_{k=1}^{n} \neg C_k(i)$$

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$$C(i) :=\blacktriangleright_j\ [j < i, Q_\#(j) \wedge \neg C_{1\to 0}(j) \wedge \neg C_{+1}(j)]0 : C_{1\to 0}(i) \vee C_{+1}(i).$$

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$$C_{+1}(i) :=\blacktriangleright_j\ [j < i, Q_\#(j)] \bigvee_{k=1}^{n} \left(\bigwedge_{r=1}^{k-1} \neg C_r(i) \wedge C_r(j) \right) \wedge C_k(i) \wedge \neg C_k(j) \wedge \left(\bigwedge_{r=k+1}^{n} C_r(i) \leftrightarrow C_r(j) \right) : 0$$

$$C_{1\to 0}(i) :=\blacktriangleright_j\ [j < i, Q_\#(j)] \bigwedge_{k=1}^{n} \neg C_k(i) \wedge C_k(j) : \bigwedge_{k=1}^{n} \neg C_k(i)$$

$$C(i) :=\blacktriangleright_j\ [j < i, Q_\#(j) \wedge \neg C_{1\to 0}(j) \wedge \neg C_{+1}(j)]0 : C_{1\to 0}(i) \vee C_{+1}(i).$$

Require $C(|enc(\tau)|) = 1$.

The construction: final tile checking

Example

$0000a_1\#0001a_2\#0010a_3\#\cdots\#1111a_{2^4}\#$. ($n = 4$, $m = 1$ and $a_i \in T$ for $i \in [2^4]$.)

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$$B_t(i) :=\blacktriangleright_j \left[j < i, \bigvee_{t' \in T} Q_{t'}(j) \right] Q_t(j) : 0 \qquad \text{for all } t \in T$$

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$$F(i) := Q_{\#}(i) \wedge B_{t_{fin}}(i) \wedge \bigwedge_{k=1}^{n} C_k(i).$$

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The construction: boundary checking (1)

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$$E_\perp(i) :=\blacktriangleright_j \left[j < i, Q_\#(j) \wedge \bigwedge_{k=1}^{n} C_k(i) \leftrightarrow C_k(j) \right] 1 : \bigvee_{\substack{t \in T: \\ down(t)=0}} B_t(i)$$

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$$\left(\bigvee_{\substack{t\in T:\\ up(t)=0}} B_t(j) \right) \wedge \left(\bigvee_{\substack{t\in T:\\ up(t)=0}} B_t(i) \right) : 0$$

The construction: boundary checking (2)

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$$E_{\vdash}(i) := \left(\bigwedge_{k=1}^{n} \neg C_k(i)\right) \to \left(\bigvee_{\substack{t\in T:\\ left(t)=0}} B_t(i)\right)$$

$$E_{\dashv}(i) := \left(\bigwedge_{k=1}^{n} C_k(i)\right) \to \left(\bigvee_{\substack{t\in T:\\ right(t)=0}} B_t(i)\right)$$

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$$E(i) :=\blacktriangleright_j [j < i, Q_{\#}(j) \wedge \neg (E_{\perp}(j) \wedge E_{\vdash}(j) \wedge E_{\dashv}(j))]$$
$$0 : E_{\perp}(i) \wedge E_{\top}(i) \wedge E_{\vdash}(i) \wedge E_{\dashv}(i).$$

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Require $E(|enc(\tau)|) = 1$.

The construction: adjacency checking

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$$M_{\downarrow}(i) :=\blacktriangleright_j \left[j < i, Q_{\#}(j) \wedge \bigwedge_{k=1}^{n} C_k(i) \leftrightarrow C_k(j) \right] \bigvee_{\substack{t,t' \in T: \\ down(t)=up(t')}} B_t(i) \wedge B_{t'}(j) : 1$$

$$M_{\leftarrow}(i) :=\blacktriangleright_j [j < i, Q_{\#}(j)] \left(\bigvee_{k=1}^{n} C_k(i) \right) \rightarrow \left(\bigvee_{\substack{t,t' \in T: \\ left(t)=right(t')}} B_t(i) \wedge B_{t'}(j) \right) : 1$$

$$M(i) :=\blacktriangleright_j [j < i, Q_{\#}(j) \wedge \neg (M_{\downarrow}(j) \wedge M_{\leftarrow}(j))]\, 0 : M_{\downarrow}(i) \wedge M_{\leftarrow}(i).$$

Require $M(|enc(\tau)|) = 1$.

The construction: wrap up

Definition (Accpetance of the B-RASP program)

1. The output vector is defined by the conjunction

$$Y(i) := A(i) \wedge C(i) \wedge F(i) \wedge E(i) \wedge M(i)$$

2. The B-RASP program accepts iff $Y(\ell) = 1$.

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- The B-RASP program recognizes the set of all $enc(\tau)$ where τ satisfies the conditions above.
- The language recognized by the B-RASP program is non-empty iff the 2^n-tiling problem has a solution.
- The construction takes time polynomial in n.
- Why does this work?

Intuition & Comparison with real transformers

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B-RASP non-emptiness $\leq_p$ UHAT non-emptiness

Formal statement

Lemma (B-RASP non-emptiness $\leq_p$ UHAT non-emptiness)

Given a B-RASP program $P_1, \ldots, P_m$ where every attention operation is of the form

$$P_{t+1}(i) := \blacklozenge_j \left[M(i,j),\, S(j) \wedge \bigwedge_{k \in K} P_k(i) \leftrightarrow P_k(j) \right] V(i,j) : D(i),$$

where

- $|\Sigma| \leq t < m$,
- $\blacklozenge \in \{\blacktriangleleft, \blacktriangleright\}$,
- $S(j)$ *is a Boolean combination of* $\{P_1(j), \ldots, P_t(j)\}$, *and*
- $K \subseteq \{1, \ldots, t\}$,

one can construct in polynomial time a UHAT that recognizes the same language.

Recap on UHAT: Masked Unique Hard-Attention (UHA)

$a_1 \quad a_2 \quad a_3 \quad a_4 \quad a_5 \quad a_6 \quad a_7$

Definition (Sketching UHA)

- Input sequence $a_1 \cdots a_n \in \Sigma^n$.

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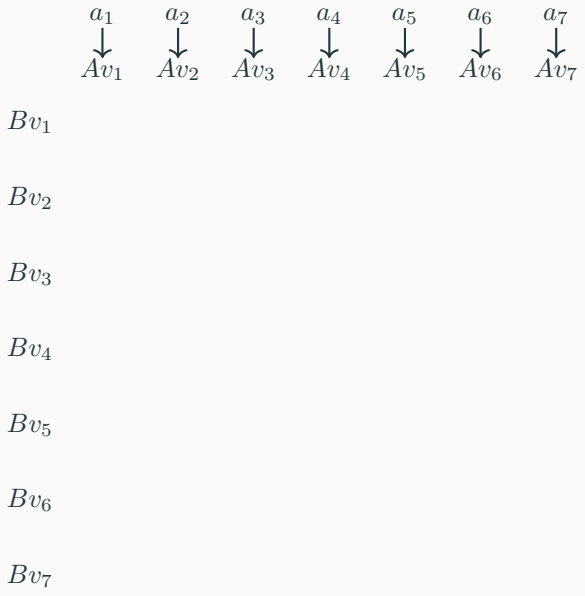

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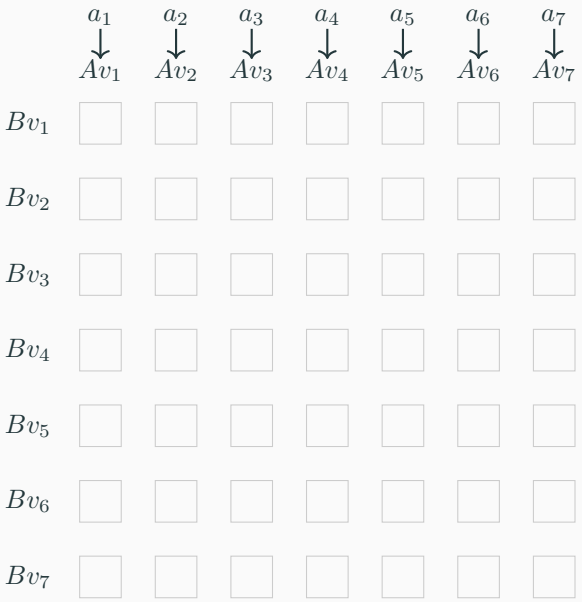

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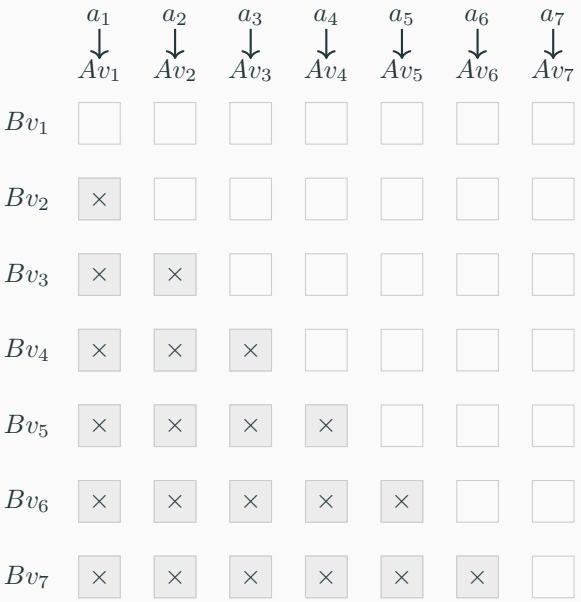

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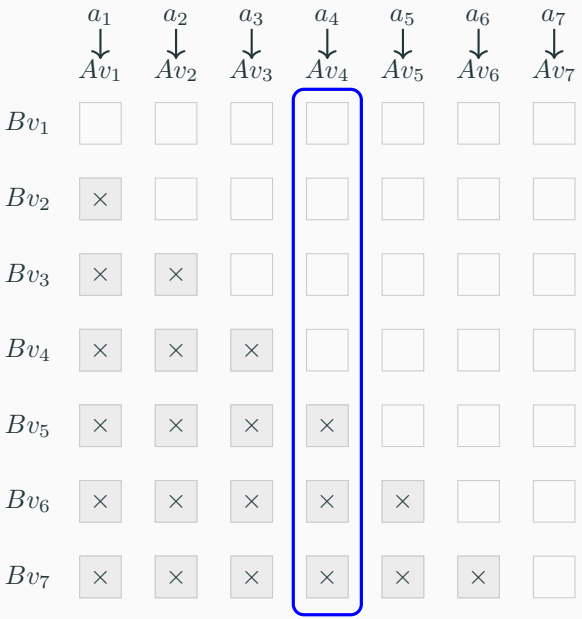

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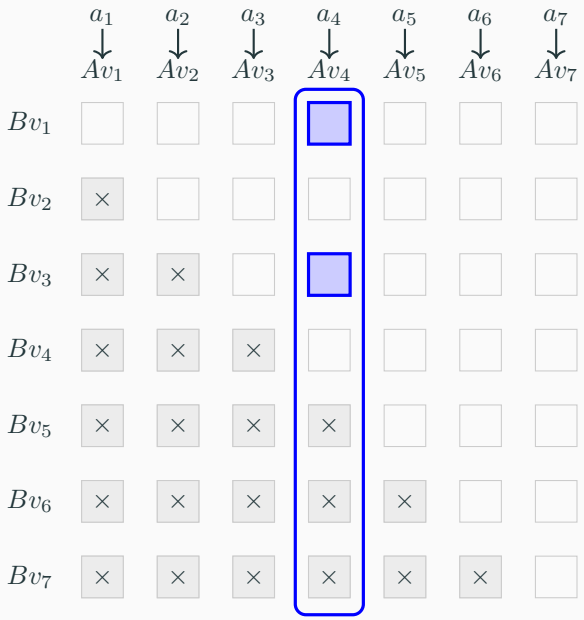

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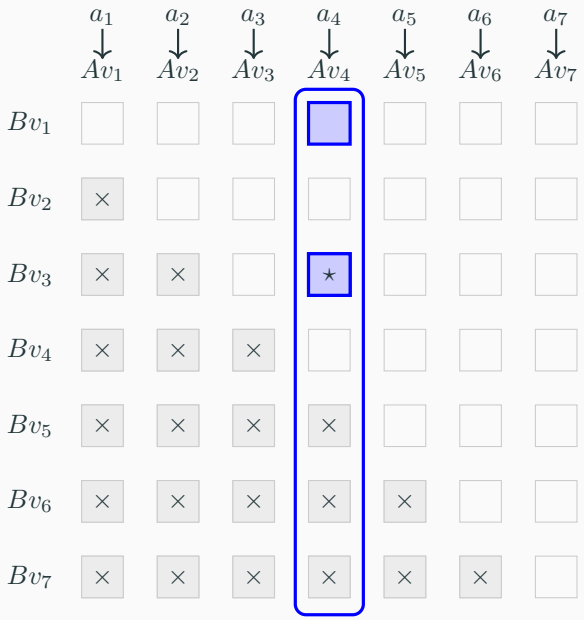

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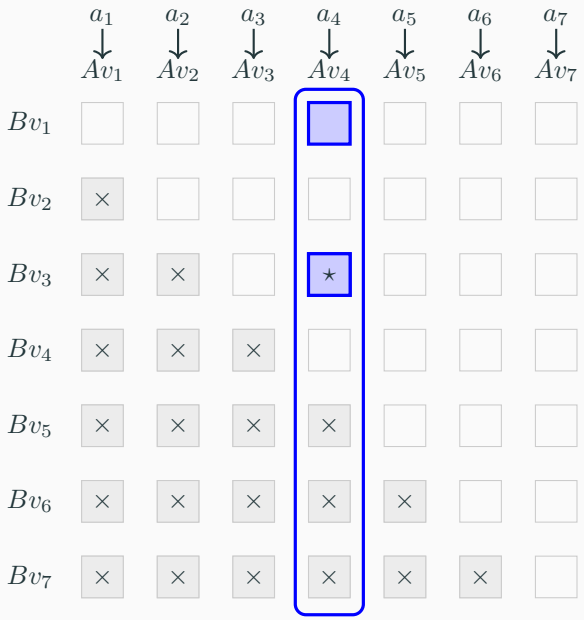
- Tie Breaking τ. (why?)
- Value Update $C : \mathbb{Q}^{2r} \to \mathbb{Q}^s$.
  For example, $v'_4 = C(v_3, v_4)$.



Recap on UHAT: ReLU, UHAT, and UHAT Acceptance

Definition (ReLU)

For each vector $v_i (i \in [n])$ and some k,

$$\mathrm{ReLU}(v_i) = (v_i[1, k-1], \max\{0, v_i(k)\}, v_i[k+1, n]).$$

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A *masked unique hard-attention transformer* (UHAT) is a length-preserving function $\mathcal{T} : \Sigma^+ \to (\mathbb{Q}^s)^+$ defined by application of a token embedding followed by application of a fixed sequence of UHA layers and ReLU layers of matching width.

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Definition (UHAT Acceptance)

Assume that $\mathcal{T}$ is given together with an *acceptance vector* $t \in \mathbb{Q}^s$. The recognized language $L(\mathcal{T})$ is then the set of words on which $\mathcal{T}$ outputs a sequence $v_1, \ldots, v_n \in \mathbb{Q}^s$ with $\langle t, v_k \rangle > 0$, where $k \in [1, n]$ is either 1 or n depending on whether the first or last position is regarded the *output position* of $\mathcal{T}$.

B-RASP Program $\rightarrow$ UHAT: Embedding and Point-Wise Operation

Embedding

Each token $a \in \Sigma$ is embedded as a one hot vector according to Q_{a_i}'s.

	1	2	3	4	5
input w	a	b	b	a	c
$P_1(Q_a)$	1	0	0	1	0
$P_2(Q_b)$	0	1	1	0	0
$P_3(Q_c)$	0	0	0	0	1
P_4	0	1	0	0	0

P_4: position i is the first b.

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Point-wise operation

- Formally, for some Boolean combination R, we set $P_{t+1}(i) := R(P_1(i), \ldots, P_t(i))$.
- In the B-RASP to UHAT translation, such Boolean combinations are simulated using affine transformations and ReLU layers.

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Simulating position-wise B-RASP operations

Bottom-up simulation needing only $\neg$ and $\wedge$

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Disjunction is obtained by De Morgan:

$$x \vee y = \neg(\neg x \wedge \neg y).$$

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and, for Boolean $x, y \in \{0, 1\}$,

$$x \wedge y = \max\{0, x + y - 1\}.$$

Disjunction is obtained by De Morgan:

$$x \vee y = \neg(\neg x \wedge \neg y).$$

After computing the subformulas of R, the UHAT keeps only

$$(P_1(i), \ldots, P_t(i), P_{t+1}(i)).$$

Restricted B-RASP attention operations

Attention Operations

$$P_{t+1}(i) := \blacktriangleright_j \left[M(i,j), S(j) \wedge \bigwedge_{k \in K} P_k(i) \leftrightarrow P_k(j) \right] V(i,j) : D(i),$$

or the analogous leftmost version.
Here: $M(i,j)$ is the mask, $S(j)$ is a Boolean condition on the candidate source position j, and

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Goal

Make UHAT hard attention select exactly the same j as the B-RASP operation.

Encoding the B-RASP score as a UHAT score

For each $k \in K$, the UHAT stores both

$$P_k(x) \qquad \text{and} \qquad 1 - P_k(x)$$

at every position x.
Use the attention score

$$\text{score}(i, j) = \sum_{k \in K} (P_k(i)P_k(j) + (1 - P_k(i))(1 - P_k(j))) - (1 - S(j)).$$

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For Boolean values,

$$P_k(i)P_k(j) + (1 - P_k(i))(1 - P_k(j)) = \begin{cases} 1, & P_k(i) = P_k(j), \\ 0, & P_k(i) \neq P_k(j). \end{cases}$$

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$$\text{score}(i, j) = |\{k \in K : P_k(i) = P_k(j)\}| - (1 - S(j)).$$

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$$\text{score}(i, j) = |\{k \in K : P_k(i) = P_k(j)\}| - (1 - S(j)).$$

The maximum possible score is $|K|$, attained exactly when

$$S(j) = 1 \quad \text{and} \quad P_k(i) = P_k(j) \text{ for all } k \in K.$$

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$$R(i) := S(j_i) \wedge \bigwedge_{k \in K} P_k(i) \leftrightarrow P_k(j_i).$$

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$$P_{t+1}(i) = \big(R(i) \wedge V(i, j_i)\big) \vee \big(\neg R(i) \wedge D(i)\big).$$

Thus:

$$R(i) = 1 \quad \Rightarrow \quad P_{t+1}(i) = V(i, j_i),$$

while

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This exactly matches the B-RASP semantics.

Preserving acceptance

The UHAT simulation maintains the invariant:

$$\text{after simulating } P_1, \ldots, P_t, \quad \text{position } i \text{ stores } (P_1(i), \ldots, P_t(i)).$$

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Acceptance

If P_t is the B-RASP output vector, stop constructing, and use acceptance one-hot vector e_t and the same output position k as P_t.
Then the UHAT accepts iff

$$\langle e_t, (P_1(k), \ldots, P_t(k)) \rangle > 0.$$

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Therefore the UHAT recognizes exactly the same language as the B-RASP program.

Questions?