

# Algorithms for Text Generation

The awes and mysteries of **generate**

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# Goal and Motivations

## Understanding Contextual Generation is Key

- LLMs are multitask learners & problem solvers via **prompting**
- evaluation of **linguistic abilities** of LLMs requires generation wrt. agreement, proper word order, semantic consistency etc.
- **good artificial data** helps ML  
privacy, confidentiality, distillation / data augmentation, artificial text detection
- computation of expectations  $\mathbb{E}_{w_{[1:T]} \sim P}(f(w_{[1:T]}))$  requires **good text samples**  
e.g., to train GANs or PPO

# Goal and Motivations

## This class

- ✓ understand the **variety of controls** for basic text generation with 🤖 **generate** as the main tool ( 🚩 **generate** has a similar, less complete interface)
  - ✓ learn to generate texts **with constraints**
  - ✓ explore some **meta-generation** algorithms
- train LLMs for better / adapted / non-autoregressive ... generation

## generate

```
model_inputs = tokenizer(["A sequence of numbers: 1, 2"], return_tensors="pt").to("cuda")
```

```
generated_ids = model.generate(**model_inputs)  
tokenizer.batch_decode(generated_ids, skip_special_tokens=True)[0]
```

```
generated_ids = model.generate(**model_inputs, max_new_tokens=50)  
tokenizer.batch_decode(generated_ids, skip_special_tokens=True)[0]
```

# Part I

## Basics

# A Language Model is a Distribution

## Language Models (LM)

Assume **finite vocabulary**  $\mathcal{V}$ , with  $\bar{\mathcal{V}} = \mathcal{V} \cup \{ \langle s \rangle, \langle /s \rangle \}$

A neural language model is a **parameterized distribution** over **complete texts** in  $\langle s \rangle \mathcal{V}^* \langle /s \rangle$  :

$$\begin{aligned} \langle s \rangle w_1 \dots w_T \langle /s \rangle &\rightarrow P(\langle s \rangle w_1 \dots w_T \langle /s \rangle | \theta) \\ \forall T > 0, \forall w_1 \dots w_T, P(\langle s \rangle w_1 \dots w_T \langle /s \rangle | \theta) &\geq 0, \\ \sum_{T, w_{[1:T]}} P(\langle s \rangle w_1 \dots w_T \langle /s \rangle | \theta) &= 1 \end{aligned}$$

Notations:

- $w_{[1:T]} = w_1 \dots w_T$
- $[w_{[1:T]}]$  assumes  $w_0 = \langle s \rangle$ , denotes a **strict prefix** (unless  $w_T = \langle /s \rangle$ )
- $[w_{[1:T]}]$  assumes  $w_{T+1} = \langle /s \rangle$ , denotes a **complete text**
- $w_{<t} : \langle s \rangle w_1 \dots w_{t-1}$
- $[w_{-t}] : \langle s \rangle \dots w_{t-1} \text{ } \overline{\text{---}} \text{ } w_{t+1} \dots w_T \langle /s \rangle$
- for  $w_T \neq \langle /s \rangle$ ,  $P([w_1 \dots w_T] | \theta)$  is a **prefix probability**
- $\sum_{w_{[1:T]}} P([w_1 \dots w_T] | \theta) = 1$  for same length prefixes

# A Language Model is a Distribution

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- $[w_{[1:T]}]$  assumes  $w_{T+1} = \langle /s \rangle$ , denotes a **complete text**
- $w_{\prec t} : \langle s \rangle w_1 \dots w_{t-1}$
- $[w_{\prec t}] : \langle s \rangle \dots w_{t-1} \_ w_{t+1} \dots w_T \langle /s \rangle$
- for  $w_T \neq \langle /s \rangle$ ,  $P([w_1 \dots w_T] \mid \theta)$  is a **prefix probability**
- $\sum_{w_{[1:T]}} P([w_1 \dots w_T] \mid \theta) = 1$  **for same length prefixes**

# Formalizing Text Generation as Search

Unconditional Text Generation: find “most likely text”

$$[w_1^* \dots w_{T^*}^*] = \operatorname{argmax}_{T, [w_{1:T}]} P([w_{1:T}] | \theta)$$

Finding  $T^*$  is part of the problem

Conditional Text Generation: find “most likely response” given input context / query (MAP)

$$[w_1^* \dots w_{T^*}^*] = \operatorname{argmax}_{T, [w_{1:T}]} P([w_{1:T}] | \mathbf{C}, \theta)$$

$\mathbf{C}$  : a prefix (**text completion**), a question (**question answering**), a source text (**translation**), a long text (**summarization**), a speech file (**transcription**), an image (**captioning**), ...

A variety of situations between **open set generation** (many acceptable texts) and **near deterministic generation** (one single acceptable output)

# Formalizing Text Generation as Search

## Unconditional Text Generation: Find the Mode

$$\begin{aligned}
 [w_1^* \dots w_{T^*}^*] &= \operatorname{argmax}_{T, [w_{1:T}]} P([w_{1:T}] | \theta) \\
 &= \operatorname{argmax}_{T, [w_{1:T}]} \prod_{t=1}^{T+1} P(w_t | w_{<t}; \theta) && \text{Chain rule for autoregressive / causal LMs} \\
 &= \operatorname{argmax}_{T, [w_{1:T}]} \log \prod_{t=1}^{T+1} P(w_t | w_{<t}; \theta) && \text{log is monotonous} \\
 &= \operatorname{argmin}_{T, [w_{1:T}]} \sum_{t=1}^{T+1} -\log P(w_t | w_{<t}; \theta) && \text{log turns } \prod \text{ into } \sum
 \end{aligned}$$

- $-\log P(w_t | w_{<t}; \theta) > 0$  is the **surprisal**; upper bounded by  $\log |\mathcal{V}|$   
quantifies how much  $w_t$  was expected given  $w_{<t}$ , used in **psycholinguistic studies**
- $\max_{T, [w_{1:T}]} P([w_{1:T}] | \theta)$  equivalently minimizes a summation of  $T + 1$  surprisals



# Formalizing Text Generation as Search

## Maximum “a posteriori” (MAP) Text Generation

$$P(w | w_{<t}; \theta) = \frac{\exp \text{logit}(w, w_{<t}; \theta)}{\sum_{w' \in \mathcal{V}} \exp \text{logit}(w', w_{<t}; \theta)}$$

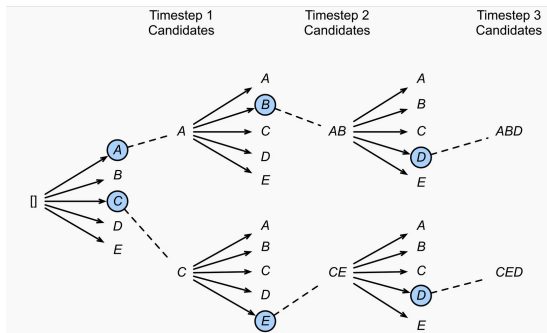
$$\log P(w | w_{<t}; \theta) = \text{logit}(w, w_{<t}; \theta) - \log \sum_{w' \in \mathcal{V}} \exp \text{logit}(w', w_{<t}; \theta)$$

$$[w_1^* \dots w_{T^*}^*] = \underset{T, [w_{1:T}]}{\operatorname{argmax}} \left( \sum_{t=1}^{T+1} \text{logit}(w_t, w_{<t}; \theta) - \log \sum_{w'} \exp \text{logit}(w', w_{<t}; \theta) \right)$$

$$= \underset{T, [w_{1:T}]}{\operatorname{argmax}} \sum_{t=1}^{T+1} \text{logit}(w_t, w_{<t}; \theta)$$

- $X$  a finite set,  $f : X \rightarrow \mathbb{R}$  a real function,  $\frac{\exp f(x)}{\sum_{x' \in X} \exp f(x')}$  is the **softmax**
- $\text{softmax}(x)$  is always  $> 0$ ; almost 1 for the largest  $f(x)$ , almost 0 otherwise
- computing the logits requires a **full forward pass** in Transformers ( $O(T \times L \times d_{\text{model}})$ )
- **normalizer**  $\sum_{w' \in \mathcal{V}} \exp \text{logit}(w', w_{<t}; \theta)$  can be expensive to compute ( $\sum$  over  $|\mathcal{V}|$  terms)

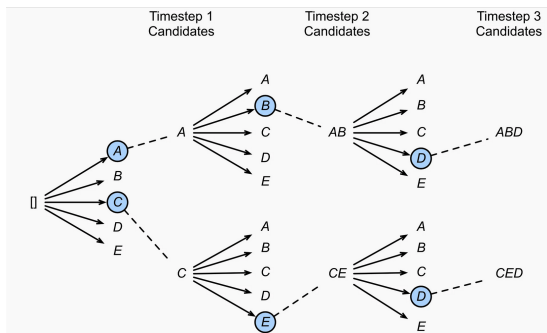
# Searching, searching, searching



source <https://towardsdatascience.com/decoding-strategies-that-you-need-to-know-for-response-generation>

- $-\log P(w_t | w_{<t}; \theta)$  **factorize** / decompose over arcs  $\Rightarrow$  **incremental score computation**
- $-\log P(w_t | w_{<t}; \theta)$  depends on the **entire prefix**  $\Rightarrow$  no DP solution
- exact search is doable [Stahlberg and Byrne, 2019], yet very costly  $\Rightarrow$  **heuristic search** (greedy, DFS, Beam,  $A^*$ , etc)

# Searching, searching, searching



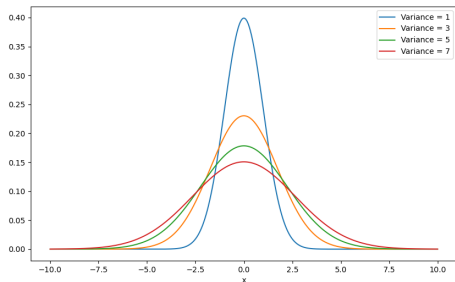
source <https://towardsdatascience.com/decoding-strategies-that-you-need-to-know-for-response-generation>

Variants and generalizations:

- restrict solutions to a strict subset of  $\langle s \rangle \mathcal{V}^* \langle /s \rangle$ : calculability and complexity issues
- use alternative, **non-decomposable** score functions  $F([w_{1:t}], \mathbf{C}; \theta)$
- use scores that **only evaluate leaf** nodes  $F([w_{1:t}], \mathbf{C}; \theta)$

# Entropies

A measure of randomness



$$H(P(T, W_{[1:T]} | \theta)) = - \sum_{T, [W_{[1:T]}]} P(T, [w_{1:T}] | \theta) \log P(T, [w_{1:T}] | \theta)$$

$$= \mathbb{E}_{T, [W_{[1:T]}] \sim P} (-\log P(T, [w_{1:T}] | \theta))$$

$$H(P(W_t | w_{<t}; \theta)) = - \sum_{w \in \mathcal{V}} P(w | w_{<t}; \theta) \log P(w | w_{<t}; \theta) \quad \text{average surprisal at time } t$$

# Entropies

A measure of randomness

## KL-Divergence

$$\begin{aligned}
 KL(P||Q) &= \sum_{w_{[1:T]}} P(T, [w_{[1:T]}] | \theta) \log \frac{P(T, [w_{[1:T]}] | \theta)}{Q(T, [w_{[1:T]}] | \theta)} \\
 &= \sum_{w_{[1:T]}} -P(T, [w_{[1:T]}] | \theta) \log Q(T, [w_{[1:T]}] | \theta) - H(P(T, [w_{[1:T]}] | \theta))
 \end{aligned}$$

- Always positive
- Null iff  $P = Q$
- Asymmetrical
- No triangle inequality
- KL is also an expectation

# Evaluating Language Models with Perplexity

Perplexity of a test sequence  $[w_{1:T}]$  [Brown et al., 1992]

$$\text{PPL}(M_{\theta}) = 2^{\frac{-1}{T} \log_2 P([w_{1:T}] | M_{\theta})} = P([w_{1:T}] | M_{\theta})^{-\frac{1}{T}}$$

Assumes “sufficiently large”  $T$ . Alt take: **normalizer** =  $T+1$ .

- The **cross-entropy** between the source ( $S$ ) and model  $M$ :

$$H(S, M_{\theta}) = \lim_{T \rightarrow \infty} \frac{-1}{T} \log_2 P([w_{1:T}] | M_{\theta})$$

$H(S, M_{\theta})$  upper bounds  $H(S)$

- PLL() **homogeneous to a vocabulary size**

$$\text{PPL}(\text{Unif}) = 2^{\frac{-1}{T} \log_2 P([w_{1:T}] | M_{\theta})} = 2^{\frac{-1}{T} T \log_2 (1/|\mathcal{V}|)} = |\mathcal{V}|$$

# Evaluating Language Models with Perplexity

PPL is hard to understand

Comparing LMs with different support or tokenizers ?

- ❶ closed-world LMs assume a fixed vocabulary size  $|\mathcal{V}|$  - models with different  $\mathcal{V}$  **cannot be compared**.
- ❷ open-world models with different **segmentations** can be compared, **must use a common normalizer**
- ❸ typical normalizers when using subwords vocabularies
  - number of chars  $\Rightarrow$  **bits per char**  $\equiv \log_2$  of char-normalized PPL
  - number of bytes  $\Rightarrow$  **bits per byte**  $\equiv \log_2$  of byte-normalized PPL

# Evaluating Language Models with Perplexity

Implementing  $\sum_{t=1}^T \log P(w_t | w_{<t}; \theta)$  with **finite, fixed-length window of size  $L$** ?

- split in short parts of length  $T_i < L$  (lines, paragraphs); average over parts;
- “reshape” text into  $\lfloor T/L \rfloor$  sequences of length  $L$ , average  $\log P(w_L | w_{<L})$  over blocks
- “reshape” text into  $T - L$  sequences of length  $L$  with shift 1, average  $\log P(w_L | w_{<L})$  over blocks;
- “reshape” text into  $\lfloor 2 \times (T - L)/L \rfloor$  sequences of length  $L$  with shift  $L/2$ , average  $\sum_{t=L/2}^L \log P(w_L | w_{<L})$  over blocks;

📄 🤖 <https://huggingface.co/docs/transformers/perplexity>

**Pros and Cons?**



# Evaluating Language Models with Perplexity

**Caveat: segmentation ambiguities and exact surprisal computations**

$$P(abcd|\theta) = \sum P(a\_bcd|\theta) + P(ab\_cd|\theta) + \dots P(abc\_d|\theta)$$

# Language model (de)generation

Language Generation is Hard

## The promise

📄 OpenAi Website <https://openai.com/blog/better-language-models/>

GPT-2 generates synthetic text samples in response to the model being primed with an arbitrary input. The model is chameleon-like—it adapts to the style and content of the conditioning text. This allows the user to generate **realistic and coherent continuations** about a topic of their choosing, as seen by the following select samples.

GPT-2 displays a broad set of capabilities, including the ability to **generate conditional synthetic text samples of unprecedented quality**, where we prime the model with an input and have it generate a lengthy continuation.

# Language model (de)generation

## The truth about language model generation

---

<b>Prefix Greedy</b>	Lyrically the song has excerpts of different languages including French , Spanish , German , Italian , Portuguese , Spanish , Portuguese , Portuguese , Portuguese , Portuguese , Portuguese , Portuguese , Portuguese , Portuguese , Portuguese , Portuguese , Portuguese , Portuguese , Portuguese , ...
<b>Top3</b>	German , Italian , Portuguese , Spanish , Portuguese , Portuguese , Italian and Spanish. It is also available in English, French and Spanish. In addition to its lyrics, the album features a number of original songs, ...
<b>Nucleus-0.3</b>	German , Italian , Portuguese , Spanish , Portuguese , Italian , Portuguese , Spanish , Portuguese , Spanish , Portuguese , Spanish , Portuguese , Spanish , Portuguese , Spanish , Portuguese , Spanish , Portuguese , ...

---

<b>Prefix Greedy</b>	The first pair of pereiopods is armed with a large , asymmetrical, and long-range laser cannon. The second pair is armed with a large , asymmetrical, and long-range laser cannon. The third pair is armed with a large , asymmetrical, and long-range laser cannon. The fourth pair is armed with a large ...
<b>Top3</b>	etrical, and highly mobile head, and the second pair has a small , asymmetrical, and highly mobile head. The second pair has a large and highly mobile head, and the third pair is armed with a large and highly mobile head. The first pair ...
<b>Nucleus-0.3</b>	etrical head and a large body. The first pair of pereiopods is armed with a large , asymmetrical head and a large body. The first pair of pereiopods is armed with a large , asymmetrical head and a large body. The first pair of pereiopods is armed ...

---

GPT-2 generated examples from [Welleck et al., 2020b].

# Language model (de)generation

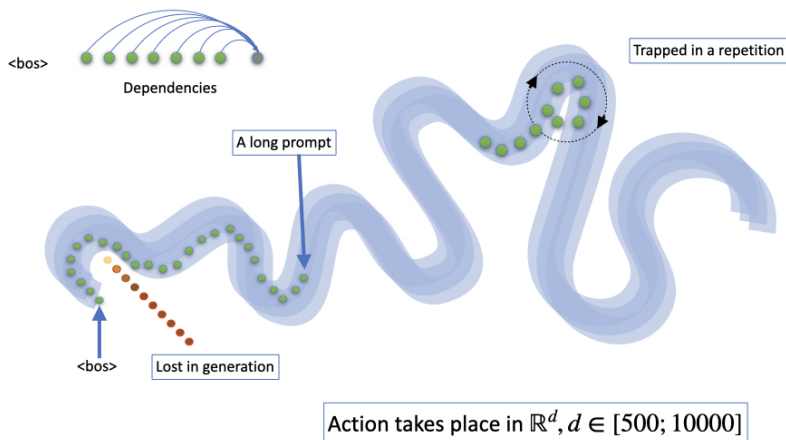
## Language Generation is Hard

### High probability sentences do not resemble human productions

- too many repetitions
- high frequency tokens over-represented, low frequency tokens under-represented
- lack of lexical diversity
- lack of global consistency
- posterior distribution poorly calibrated

# Language model (de)generation

Language Generation is Hard



# Evaluating LMs with distributional properties

**rep/ $\ell$** : a repetition / diversity metric [Welleck et al., 2020b]

Given a set  $\mathcal{D}$  of length- $T$  sequences,

$$\text{rep}/\ell = \frac{1}{|\mathcal{D}|T} \sum_{\mathbf{x} \in \mathcal{D}} \sum_{t=1}^T \mathbb{I}[\mathbf{w}_t \in \mathbf{w}_{t-\ell-1:t-1}].$$

$\mathbb{I}$  the indicator function. Generalizes to repeated n-gram sequences.

# Evaluating LMs with distributional properties

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**Global distributional properties** [Meister and Cotterell, 2021]

- Zipfian behavior, power-law distribution

$$P_{\text{zipf}}(W = w_k) \propto k^{-s}, s \approx 1$$

$w_k$  is the  $k^{\text{th}}$  most frequent token

- type-token ratios (TTR) (depends on length)
- proportion of frequency 1 words (*hapax legomena*)
- proportion specific of token classes (punctuation, stopwords etc)
- consistency metrics ?

# Evaluating LMs with distributional properties

MAUVE, a precision-recall approach [Pillutla et al., 2024]

- comparing model distribution and true distribution with KL divergence is risky due to difference of support
- safer to compute

$$Q_{\lambda}([w_{1:T}]|\theta) = \lambda P([w_{1:T}]) + (1 - \lambda) P_{\lambda}([w_{1:T}]|\theta)$$

- MAUVE score is **the area under the curve** associating  $KL(P([w_{1:T}])||Q_{\lambda}([w_{1:T}]|\theta))$  vs  $KL(P([w_{1:T}]|\theta)||Q_{\lambda}([w_{1:T}]|\theta))$  with varying  $\lambda \in [0 : 1]$  (more precisely  $\exp -KL$ ).
- use statistics in the embedding space for a fixed model (eg. GPT-2) to approximate these quantities

Discussion and comments in [Pimentel et al., 2023].



# Evaluating zero-shot / few-shot behaviour

Reduce NLP tasks to text generation with appropriate instructions in NL as prompts

Prompts = instructions in Natural Language + [tricks] (from [Brown et al., 2020])

Specifically, we evaluate GPT-3 on over two dozen NLP datasets,(...) For each task, we evaluate GPT-3 under 3 conditions:

- “**zero-shot**” learning, where no demonstrations are allowed and only an instruction in natural language is given to the model.

“Evaluate  $125 + 12 =$ ”

- “**one-shot learning**”, where we allow only one demonstration, and

“Evaluate  $17 + 301 = 318$  </s>Evaluate  $125 + 12 =$ ”

- “**few-shot learning**”, or in-context learning, where we allow as many demonstrations as will fit into the model’s context window,

“Evaluate  $17 + 301 = 318$  </s>Evaluate  $48 + 67 = 105$  </s>Evaluate  $125 + 12 =$ ”

Tricks: “On tasks with free-form completion, we use beam search with the same parameters as [RSR+19]: a beam width of 4 and a length penalty of  $\alpha = 0.6$ .” (+ stopping criterion)

# Evaluating zero-shot / few-shot behaviour

Reduce NLP tasks to text generation with appropriate instructions in NL as prompts

## Task types and their evaluation [Biderman et al., 2024]

Assuming prompt / instruction:  $w_1 \dots w_T$ .

- Yes / No answers

Question: [Question] True or false? [prediction]

Correct if  $P(\text{True} | \text{prompt}) > P(\text{False} | \text{prompt})$ .

- Multiple choice answers.

Question: Which factor will most likely cause a person to develop a fever?

Correct Answer	a bacterial population in the bloodstream
Incorrect Answer	a leg muscle relaxing after exercise
Incorrect Answer	several viral particles on the skin
Incorrect Answer	carbohydrates being digested in the stomach

Correct if  $P(\text{Correct answer} | \text{prompt}) > P(\text{Alternative} | \text{prompt})$  Alt. take - index choices with letter or numbers, evaluate the probability of the correct index.

- One word continuation. Correct if  $(w_{T+1} == w^*)$
- Multiple word continuation. Measure  $\Delta(w_{T+1} \dots w_{T+S}; w_1^* \dots w_L^*)$  with  $\Delta()$  task-dependent distance (ROUGE for summarization, BLEU for MT, etc)

# Evaluating zero-shot / few-shot behaviour

Reduce NLP tasks to text generation with appropriate instructions in NL as prompts

## Understanding “instruction learning” results

Should pay attention to:

- how much effort went into prompting ?
- free generation or text infilling or multi-choice answers ?
- how were alternatives selected / generated ?
- how was search performed (greedy or beam ) ?
- how does generation stops
- how many shots is few shots?

## Open issues

- generating / optimizing discrete / continuous prompts
- training with prompts and meta-learning

## Part II

# Algorithms for Text Generation

# Deterministic Algorithms for Text Generation

Searching for the Maximum “A Posteriori”

## Greedy search (a.k.a argmax)

$$w_0 = \textcolor{blue}{<s>}$$

$$\forall t > 0, w_t = \operatorname{argmax}_{w \in \bar{\mathcal{V}}} \log P(w | w_{<t})$$

$$\bar{\mathcal{V}} = \mathcal{V} \cup \{\textcolor{blue}{<s>}, \textcolor{blue}{</s>}\}$$

Generation stops with  $\textcolor{blue}{</s>}$  or when some maximum length  $T_{\max}$  is reached.

- Greedy search is **deterministic**: always produces the same output, given its initial conditions.
- Does not require to compute softmax normalizer  $\log(\sum \exp())$

# Deterministic Algorithms for Text Generation

Searching for the Maximum “A Posteriori”

## Beam search [with histogram pruning]

$$W_0 = \{ \langle s \rangle \}$$

$$\forall t > 0, W_t = \underset{\substack{W'_t \subseteq \mathcal{B}_t, \\ |W'_t| = k}}{\operatorname{argmax}} \mathcal{L}(W'_t)$$

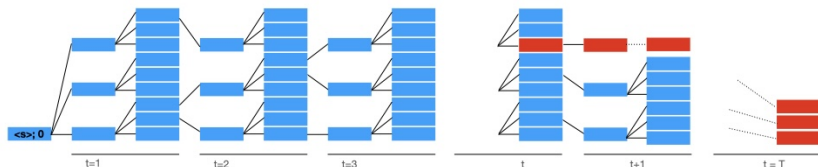
where  $\mathcal{B}_t$  is the **beam**, consisting of all possible extensions of  $W_{t-1}$ .

$\mathcal{L}: \mathcal{W} \rightarrow \mathbb{R}$  is a scoring function that operates over sets  $W \subseteq \mathcal{W}$ , eg.  $\mathcal{L}(W) = \sum_{w_{[1:t]} \in W} \log P(w_{[1:t]})$ .

- For  $k = 1$ , beam search is greedy search
- For  $k > 1$ , **does require** to compute softmax normalizer  $\log(\sum \exp())$ . Why ?
- Also: adaptive beam size, with  $\mathcal{B}_t$  containing all outputs with score within  $\alpha$  % of the current best.
- A faster version borrowing ideas from  $A^*$  search [Meister et al., 2020b]
- 🤖 generate:  $k = \text{num\_beams}$

# Deterministic Algorithms for Text Generation

Searching for the Maximum “A Posteriori”



## Vanilla Beam stopping condition

$$([w_{[1:t]}^*, s_t^*] = \operatorname{argmax}_s \mathcal{B}_t, w_t^* = \text{</s>})$$

In words: the top hypothesis in the beam is **complete**.

# Deterministic Algorithms for Text Generation

Flavors of Beam Search - Delivering  $k$  solutions [Kasai et al., 2024]

$k$ : beam size,  $M$ : maximum length,  
 $\mathcal{V}$ : Vocabulary,  $\text{score}(\cdot)$ : scoring function.

```

1:  $B_0 \leftarrow \{\langle 0, \langle s \rangle \rangle\}$ 
2: for  $t \in \{1, \dots, M-1\}$  do
3:   for  $\langle s, w_{[1:t]} \rangle \in B_{t-1}$  do
4:     if  $w_t = \langle /s \rangle$  then
5:        $H.\text{add}(\langle s, w_{[1:t]} \rangle)$ 
6:       continue
7:     end if
8:     for  $w \in \mathcal{V}$  do
9:        $s \leftarrow \text{score}(w_{[1:t]} \circ w)$ 
10:       $H.\text{add}(\langle s, w_{[1:t]} \circ w \rangle)$ 
11:    end for
12:  end for
13:   $B_t \leftarrow \emptyset$ 
14:  while  $|B_t| < k$  do
15:     $\langle s, w_{[1:t]} \rangle \leftarrow H.\text{max}()$ 
16:     $B_t.\text{add}(\langle s, w_{[1:t]} \rangle)$ 
17:     $H.\text{remove}(\langle s, w_{[1:t]} \rangle)$ 
18:  end while
19:  if  $\forall w_{[1:t]} \in B_t, w_t = \langle /s \rangle$  then break
20:  end if
21: end for
22: return  $B_t.\text{max}()$ 

```

- Implementing  $H$  as a **Heap**, operations (add, remove, max) take  $O(\log |\mathcal{V}|)$
- 🤖 generate `num_beams ( $k$ )`,  
`num_return_sequences`
- the stopping condition is 🤖 generate  
`early_stopping = True` (also `False`,  
`never`)



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8:     for  $w \in \mathcal{V}$  do
9:        $s \leftarrow \text{score}(w_{[1:t]} \circ w)$ 
10:       $H.\text{add}(\langle s, w_{[1:t]} \circ w \rangle)$ 
11:    end for
12:  end for
13:   $B_t \leftarrow \emptyset$ 
14:  while  $|B_t| < k$  do
15:     $\langle s, w_{[1:t]} \rangle \leftarrow H.\text{max}()$ 
16:     $B_t.\text{add}(\langle s, w_{[1:t]} \rangle)$ 
17:     $H.\text{remove}(\langle s, w_{[1:t]} \rangle)$ 
18:  end while
19:  if  $\forall w_{[1:t]} \in B_t, w_t = \langle /s \rangle$  then break
20:  end if
21: end for
22: return  $B_t.\text{max}()$ 

```

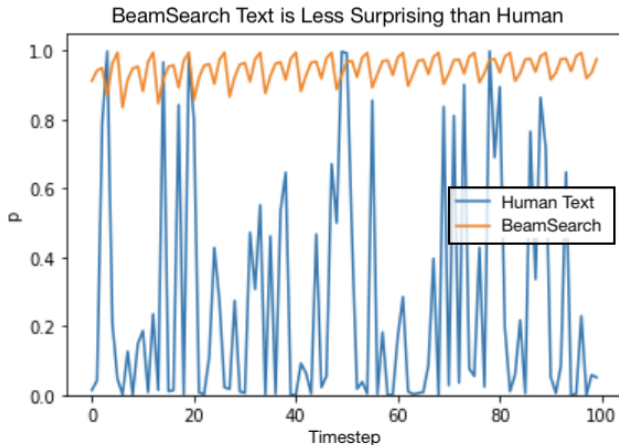
$k$ : beam size,  $M$ : maximum length,  $p$  patience  
 $\mathcal{V}$ : Vocabulary,  $\text{score}(\cdot)$ : scoring function.

```

1:  $B_0 \leftarrow \{\langle 0, \langle s \rangle \rangle\}, F_0 \leftarrow \emptyset$ 
2: for  $t \in \{1, \dots, M-1\}$  do
3:    $H \leftarrow \emptyset, F_t \leftarrow F_{t-1}$ 
4:   for  $\langle s, w_{[1:t]} \rangle \in B_{t-1}$  do
5:     for  $w \in \mathcal{V}$  do
6:        $s \leftarrow \text{score}(w_{[1:t]} \circ w)$ 
7:        $H.\text{add}(\langle s, w_{[1:t]} \circ w \rangle)$ 
8:     end for
9:   end for
10:   $B_t \leftarrow \emptyset$ 
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12:     $\langle s, w_{[1:t]} \rangle \leftarrow H.\text{max}()$ 
13:    if  $w_t = \langle /s \rangle$  then
14:       $F_t.\text{add}(\langle s, w_{[1:t]} \rangle)$ 
15:    else
16:       $B_t.\text{add}(\langle s, w_{[1:t]} \rangle)$ 
17:    end if
18:     $H.\text{remove}(\langle s, w_{[1:t]} \rangle)$ 
19:  end while
20:  if  $|F_t| = pk$  then break
21:  end if
22: end for
23: return  $F_t.\text{max}()$ 

```

# Pitfalls of Beam Search



From <https://huggingface.co/blog/how-to-generate>

Also [Holtzman et al., 2020]. This can make **artificial text detection** easy.

# Pitfalls of Beam Search

## The Beam Search “curse”

Russian–English (medium)	Beam Size					
	10	50	75	100	150	1000
BLEU	24.9	23.8	23.6	23.3	22.5	3.7
METEOR	30.9	30.0	29.7	29.4	28.8	12.8
length	0.90	0.86	0.85	0.84	0.81	0.31

Results of the Russian–English translation system. We report BLEU and METEOR scores, as well as the ratio of the length of generated sentences compared to the correct translations (length). From [Murray and Chiang, 2018]

**Increasing beam width  $k$  hurts performance (!)**

# Pitfalls of Beam Search

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## Increasing beam width $k$ hurts performance (!)

### Length issues in beam search

- Increasing  $k$  raises the likeliness of inserting a complete hypothesis in  $\mathcal{B}_t$
- Complete hypotheses scores do not change;
- **Uncomplete hypotheses scores only gets worse**
- Short sequences are more likely than longer ones

**The problem is the MAP not the beam [Eikema and Aziz, 2020] ! Small beams hide this issue**

# Pitfalls of Beam Search

Better solutions with regularized decoding objectives [Meister et al., 2020a]

$$[w_1^* \dots w_{T^*}^*] = \operatorname{argmin}_{T, w_{[1:T]}} \sum_{t=1}^{T+1} -\log P(w_t | w_{<t}; \theta) - \lambda \mathcal{R}([w_{[1:T]}])$$

$\mathcal{R}([w_{[1:T]}])$  compensates for length differences, biases towards longer sequences

- 1  $\mathcal{R}([w_{[1:T]}]) = T + 1$ : fixed bonus for each extra word  
~ score with **average surprisal**  $\frac{1}{T+1} \sum_{t=1}^T -\log P(w_t | w_{<t}; \theta)$
- 2  $\mathcal{R}_{\text{unif}}([w_{[1:T]}]) = \frac{1}{T} \sum_t (\log P(w_t | w_{<t}; \theta) - \mu_t)^2$ , with  $\mu_t$  average surprisal  
enforces **uniform information rate**
- 3  $\mathcal{R}_{\text{local}}([w_{[1:T]}]) = \frac{1}{T+1} \sum_t (\log P(w_t | w_{<t}; \theta) - \log P(w_{t-1} | w_{<t-1}; \theta))^2$ ,  
enforces **locally uniform information rate**
- 4  $\mathcal{R}_{\text{max}}([w_{[1:T]}]) = \frac{1}{T+1} \max_t (-\log P(w_t | w_{<t}; \theta))$ ,  
enables **high surprisal tokens**

- 🗨 generate with `length_penalty= $\lambda$`  to control output length

# Pitfalls of Beam Search

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 enables **high surprisal tokens**

- 🤖 generate with `length_penalty= $\lambda$`  to control output length

# Sampling Schemes for Text Generation

## Ancestral sampling

$$w_0 = \text{<s>}$$

$$\forall t > 0, w_t \sim P(w | w_{<t}; \theta)$$

Recursion stops with `</s>` or when some maximum length  $T_{\max}$  is reached.

- Ancestral sampling is **non-deterministic**: output varies, depending on the sharpness of  $P(w | w_{<t}; \theta)$
- Sampling requires 🤖 **generate** `do_sampling=True`
- softmax is very peaked: increase diversity with **temperature**  $\tau$  to “flatten” the distribution with  $\exp \frac{\text{logit}(w', w_{<t}; \theta)}{\tau}$  ( $\tau$  is 🤖 **generate temperature**)
- better trade-off between likelihood and diversity [Keskar et al., 2019]:

$$P(w' | w_{<t}; \theta) \propto \exp \frac{\text{logit}(w', w_{<t}; \theta)}{\tau \times \mathbb{I}(w' \in w_{<t})},$$

with  $\mathbb{I}(w' \in w_{<t}) = 1$  for “new tokens”,  $= \lambda > 1$  for “old ones” (**repetition\_penalty** for 🤖 **generate**)

# Sampling Schemes for Text Generation

Top-k sampling [Fan et al., 2018]

$$w_0 = \text{<s>}$$

$$Q(w_t | w_{<t}) \propto \begin{cases} P(w_t | w_{<t}; \theta) & \text{if } w \in \text{top-}k(P(W | w_{<t}; \theta)) \\ 0 & \text{otherwise} \end{cases}$$

$$\forall t > 0, w_t \sim Q(w | w_{<t})$$

Sample from a “truncated” distribution containing the  $k$  most likely symbols. Generation stops with the `</s>` symbol or when some maximum time step  $T_{\max}$  is reached.

- Finding the  $k$  most likely tokens is  $O(|\mathcal{V}| * \log k)$ , the normalizer applies only over  $k$  elements.
- 🤖 - generate `top_k`



# Sampling Schemes for Text Generation

Nucleus sampling (top  $p$ , with variable  $p$ ) [Holtzman et al., 2020]

$$w_0 = \text{<s>}$$

$$Q(w_t | w_{<t}) \propto \begin{cases} P(w_t | w_{<t}; \theta) & \text{if } w \in \text{top-}p(P(W | w_{<t}; \theta)) \\ 0 & \text{otherwise} \end{cases}$$

$$\forall t > 0, w_t \sim Q(w | w_{<t})$$

$p$  is the **smallest integer such that**  $\sum_{w \in \text{top-}p} P(w | w_{<t}; \theta) > \alpha$ . Sample from a “truncated” distribution for the  $p$  most likely symbols, with variable  $p$  ( $\alpha$  typically  $\in [0.7; 0.9]$ ).

- $\alpha$  controls the size of the truncated vocabulary ( $Q(w | w_{<t}) > 0$ ).
- 🤖 - generate top\_

# Sampling Schemes for Text Generation

## Locally Typical Sampling [Meister et al., 2023]

$$w_0 = \text{<s>}$$

$$Q(w_t | w_{<t}) \propto \begin{cases} P(w_t | w_{<t}; \theta) & \text{if } w \in \text{LTStop-p}(P(W | w_{<t}; \theta)) \\ 0 & \text{otherwise} \end{cases}$$

$$\forall t > 0, w_t \sim Q(w | w_{<t})$$

LTStop-p( $P(W | w_{<t}; \theta)$ ) minimize  $\sum |H(W | w_{<t}; \theta) + \log P(w | w_{<t}; \theta)|$  subject to  $\sum_{w \in \text{LTStop-p}} P(w | w_{<t}; \theta) > \alpha$ . Sample from a “truncated” distribution for the  $p$  most **locally typical** symbols, with variable  $p$  ( $\alpha$  typically  $\in [0.7; 0.9]$ ).

- Locally typical prefers tokens with **average surprisal**
- In low uncertainty contexts, prefer high probability tokens
- In high uncertainty contexts, pick token with near average surprisal (=information content)
- 🤗 generate: `typical_p`
- related: Mirostat [Basu et al., 2021], sample with a target perplexity.

# Sampling Schemes for Text Generation

Top- $k$ , top- $p$  and typical sample from a **truncated distribution**  $Q(W \mid <_t; \theta)$ :

- $\forall t$ , select vocabulary  $\mathcal{V}_t^+ \subset \mathcal{V}$ .
- $\forall t, w \notin \mathcal{V}_t^+, Q(w \mid <_t; \theta) = 0$

Always sampling high probability words avoids derailing, yet, can be **very risky**:

- 1 generation may no longer terminate  $\Rightarrow$  probability leakage to infinite strings.
- 2 may **exclude interesting words**  
Using top- $p$ , for  $p = 0.9$ ,  $P(\text{Duck} \mid \text{Donald}) = 0.95$  excludes  $w = \text{Trump}$
- 3 may **include unlikely words**  
Using top- $k$ ,  $k = 20$  may generate unlikely continuations for low-entropy distributions

# Sampling Schemes for Text Generation

Top- $k$ , top- $p$  and typical sample from a **truncated distribution**  $Q(W | <_t; \theta)$ :

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- 3 may **include unlikely words**  
Using top- $k$ ,  $k = 20$  may generate unlikely continuations for low-entropy distributions

## Remedies

- solve (1) with **consistent truncated sampling** [Welleck et al., 2020a]:  $\mathcal{V}_t^+ \rightarrow \mathcal{V}_t^+ \cup \{</s>\}$
- how to mitigate (2) and (3) ? what is the right size for  $\mathcal{V}_t^+$  ?
  - (P1) never truncate high probability words  $\Leftrightarrow$  keep all  $w$  such that  $P(w | w_{<t}) > \epsilon; \theta$
  - (P2) truncate more when entropy is low; truncate less when entropy is high
  - (P\*) sample only  $w$  for which **the true  $P(w | <_t; \theta)$  is provably  $> 0$**  (with rejection sampling) [Finlayson et al., 2024]

# Sampling Schemes for Text Generation

$\eta$ -Sampling [Hewitt et al., 2022]

$$w_0 = \langle s \rangle$$

$$Q(w_t | w_{<t}) \propto \begin{cases} P(w_t | w_{<t}; \theta) & \text{if } w \in \mathcal{V}_t^+ \\ 0 & \text{otherwise} \end{cases}$$

$$\forall t > 0, w_t \sim Q(w | w_{<t})$$

$$\mathcal{V}_t^+ = \{w \in \mathcal{V} | P(w | w_{<t}; \theta) \geq \min(\epsilon, \alpha \exp -H(W_t | w_{<t}; \theta))\}$$

Sample from a “truncated” distribution subject to principles (P1) and (P2).

- $\alpha \exp -H(W_t | w_{<t}; \theta)$  increases the sampling set when entropy is high
- Yields better samples than typical, greedy, ancestral, nucleus and top-k
- In [Hewitt et al., 2022]’s experiments,  $\epsilon = 0.0003$ ,  $\alpha = \sqrt{\epsilon}$
- 😊 - generate `epsilon_cutoff`, `eta_cutoff`

# Consistent Decoding for Consistent Models

Why we need a maximum decoding length

Consistent model (details in [Welleck et al., 2020a])

A **consistent model** is such that  $P(|w_{[1:T]}| = \infty \mid \theta) = 0$

A sufficient condition is that **hidden states are uniformly bounded**.

This implies that  $\exists \xi, \forall t, w_{<t}, P(\text{</s>} \mid w_{<t}; \theta) > \xi$ .

$$P(|w_{[1:T]}| = \infty \mid \theta) < (1 - \xi)^T$$

$$\lim_{T \rightarrow \infty} (1 - \xi)^T = 0$$

# Consistent Decoding for Consistent Models

Why we need a maximum decoding length

## Consistent decoding algorithm

A consistent decoding algorithm generates a complete text with probability 1.

## Unconsistency of Decoding

Ancestral **is consistent**, greedy, beam, top-k, nucleus, typical, etc. **are not consistent**.

Argument: no guarantee that  $\langle /s \rangle$  will ever appear in the top-k, top-p, etc.

## Consistent Decoding for Deterministic Search

$$w_0 = \langle s \rangle$$

$$Q(w_t | w_{<t}; \theta) \propto \begin{cases} 1 - \alpha(h_t) & \text{if } w = \langle /s \rangle \\ \frac{\alpha(h_t) \exp \logit(w, w_{<t}; \theta)}{\sum_{w'} \exp \logit(w', w_{<t}; \theta)} & \text{otherwise} \end{cases}$$

$$\alpha(h_0) = \sigma(\logit(\langle /s \rangle, \langle s \rangle; \theta)) \quad (1)$$

$$\alpha(h_t) = \sigma(\logit(\langle /s \rangle, w_{<t}; \theta))(1 - P(\langle /s \rangle | w_{<t}; \theta)) \quad (2)$$

With  $\sigma : \mathbb{R} \rightarrow [0; 1 - \epsilon]$ ,  $\epsilon > 0$ ,  $\epsilon < 1$ . This ensures that  $Q(\langle /s \rangle | w_{<t}; \theta)$  is monotonically increasing, meaning that  $\langle /s \rangle$  eventually happen.

# Promoting Diversity in Text Generation

## Diversity promotion has many forms

- 1 boosting surprisal in open-ended text generation
- 2 ensuring diversity in a set of solutions
- 3 mitigating repetition in texts (difficult - repetition can be a good thing)



# Promoting Diversity in Text Generation

Boosting surprisal in open-ended text generation

## Contrasting Expert and Amateur Models

New search objective:

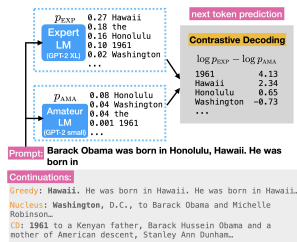
$$w_1^* \dots w_{T^*}^* = \operatorname{argmax}_{T, w_{[1:T]}} \sum_{t=1}^T \log P(w_t | w_{<t}; \theta) - \log P(w_t | w_{<t}; \theta_{AMA})$$

subject to  $\forall t, w_t^* \in \mathcal{V}_t^+$

$$\mathcal{V}_t^+ = \{w \in \mathcal{V} | P(w | w_{<t}; \theta) \geq \alpha \max_{w'} P(w' | w_{<t}; \theta)\}$$

Select probable words **that are unlikely for a weaker amateur model**.

Constraining the search to high probability words helps handle cases where (a) Expert and Amateur agree on very low probability; (b) Expert and Amateur agree on very high probability. Also respects (P1).



From [Li et al., 2023]

- requires consistent tokenization for expert and amateur
- see also: <https://arxiv.org/pdf/2305.12675.pdf>

# Promoting Diversity in Text Generation

## Generating Multiple Diverse Solutions

### Ensuring Diversity in Beam Search

Maintains  $G$  beams  $\mathcal{B}_t^1 \dots \mathcal{B}_t^G$ , such that hypotheses in Beam  $g$  must be diverse with respect to  $\mathcal{B}_t^1 \dots \mathcal{B}_t^{g-1}$

$$\begin{aligned} \text{score}(w_{[1:l]}, g) &= \text{score}(w_{[1:l]}) \text{ if } g = 1 \\ &= \text{score}(w_{[1:l]}) + \lambda \sum_{h=1}^{g-1} \Delta(w_{[1:l]}, \mathcal{B}_t^h), \text{ otherwise} \\ \Delta(w_{[1:l]}, \mathcal{B}_t^h) &= \sum_{w'_{[1:l']} \in \mathcal{B}_t^h} \delta(w_{[1:l]}, w'_{[1:l']}), \text{ with } \delta \text{ a similarity function} \end{aligned}$$

- $\Delta$  can be any string comparison (set differences for bag-of-words or bag-of-ngrams; Levenshtein distance; neural similarity, etc.)
- beams can run in parallel with a time delay
- 🤖 generate: num\_beam\_groups ( $G$ ), diversity\_penalty ( $\lambda$ )

# Promoting Diversity in Text Generation


## Avoiding Repetitions

Contrastive Search (greedy version) [Su et al., 2022]

$$w_0 = \text{<s>}$$

$$\forall t > 0, w_t = \underset{w \in \hat{\mathcal{V}}}{\operatorname{argmax}} (1 - \alpha) \log P(w | w_{<t}) - \alpha \max\{\operatorname{sim}(h_w, h_{w_s}) : 1 \leq s \leq t - 1\}$$

$h_w$  is the latent representation associated to  $w$ ;  $\operatorname{sim}$  is a similarity function (e.g. cosine). Extra penalty term for repetitions. Generation stops with `</s>` or when some maximum length  $T_{\max}$  is reached.

- assumes repetitions can be detected in embedding space
- 🤖 generate: `penalty_alpha=  $\alpha$`   <https://huggingface.co/blog/introducing-csearch>
- naive version with `no_repeat_ngram_size:` disable  $n$ -gram repetition
- 😊 DoLa contrasts inner vs. outer layers to increase factuality [Chuang et al., 2024]

# Faster Generation with Speculative Sampling

Details in [Leviathan et al., 2023] and [Chen et al., 2023]

## Overview

- Sampling algorithms are autoregressive: they return one sample at each time step.
- At step  $t$  speculative sampling uses a **simpler model** to generate  $S$  **draft tokens**  $w_{t+1} \dots w_{t+S}$  autoregressively, then “validates” the tokens with the large model **in parallel** with accept / reject procedure.
- Why? Potential to **validate multiple tokens** in one parallel forward pass.

```
[START] japan ' s benchmark bond n
[START] japan ' s benchmark nikkei 22 5
[START] japan ' s benchmark nikkei 225 index rose 22 6
[START] japan ' s benchmark nikkei 225 index rose 226 . 69 points
[START] japan ' s benchmark nikkei 225 index rose 226 . 69 points , or 0 1
[START] japan ' s benchmark nikkei 225 index rose 226 . 69 points , or 1 . 5 percent , to 10 , 9859
[START] japan ' s benchmark nikkei 225 index rose 226 . 69 points , or 1 . 5 percent , to 10 , 989 . 79 in
[START] japan ' s benchmark nikkei 225 index rose 226 . 69 points , or 1 . 5 percent , to 10 , 989 . 79 in tokyo late
[START] japan ' s benchmark nikkei 225 index rose 226 . 69 points , or 1 . 5 percent , to 10 , 989 . 79 in late morning trading , [END]
```

Figure from Leviathan et al. [2023],  $K > 4$

🤖 generate: assistant\_model (assistant\_tokenizer)

# Faster Generation with Speculative Sampling

Details in [Leviathan et al., 2023] and [Chen et al., 2023]

```

1: sample  $K$  drafts  $[w_{t+i}, q(w_{t+i})], i = 1 \dots K$ 
2: evaluate drafts  $[w_{t+i}, p(w_{t+i})]$ 
3: sample  $u_i \sim \text{Unif}[0 : 1], i = 1 \dots K$ 
4: accept  $\leftarrow \text{True}; i \leftarrow 1$ 
5: while accept and  $i \leq K$  do
6:   if  $q(w_{t+i}) < p(w_{t+i})$  then
7:      $i \leftarrow i + 1$  ▷ accept
8:   else if  $u_i < \frac{q(w_{t+i})}{p(w_{t+i})}$  then
9:      $i \leftarrow i + 1$  ▷ accept
10:  else
11:    accept  $\leftarrow \text{False}$  ▷ reject
12:     $\forall w, r(w) \propto (\max(0, p(w) - q(w)))$ 
13:    sample  $w_{t+i} \sim r(w)$ 
14:  end if
15: end while

```

## Notations:

- $p(w) = P(W | w_{<t}; \theta),$   
 $q(w) = Q(W | w_{<t}; \theta')$
- $\mathcal{V}_- = \{w | q(w) \leq p(w)\};$   
**undersampled tokens**
- $\mathcal{V}_+ = \{w | q(w) > p(w)\}$   
**oversampled tokens**

**Claim:** speculative sampling generates tokens under  $p(w)$

①  $w \in \mathcal{V}_+?$  accept with proba  $\frac{p(w)}{q(w)} \Rightarrow p'(w) = q(w) \times \frac{p(w)}{q(w)} = p(w)$

②  $w \in \mathcal{V}_-?$   $p'(w) = q(w)$  always accept and there is a **second chance**:

$$\forall v \in \mathcal{V}_+, p'(w) = q(v) \times (1 - \frac{p(v)}{q(v)}) \times (\frac{p(w) - q(w)}{\sum_{w' \in \mathcal{V}_-} p(w') - q(w')})$$

# Basic Watermarking with Green / Red Sampling

An original proposal from [Kirchenbauer et al., 2023]

## Sampling from a Random Subset of Words (hard take)

At each time step:

- 1 using  $w_{<t}$ , randomly split  $\mathcal{V}$  into  $\mathcal{V}(w_{<t}) \cup \mathcal{V}(w_{<t})$  of size  $\frac{|\mathcal{V}|}{2}$
- 2 sample next word from  $\mathcal{V}(w_{<t})$  using  $P(w | w_{<t}; \theta)$

Observing  $w_{[1:T]}$ :

- 1  $\forall t$ , compute  $\text{color}(w_t)$
- 2 for generated texts:  $\mathbb{E}(n_{\text{green}}) = T$
- 3 for natural text:  $\mathbb{E}(n_{\text{green}}) = \frac{T}{2}, \mathbb{V}(n_{\text{green}}) = \frac{T}{2} \Rightarrow$  effective testing procedure

**Robust to attack, also work with greedy and beam-search decoding, degrade generation quality in low surprisal contexts**

# Basic Watermarking with Green / Red Sampling

An original proposal from [Kirchenbauer et al., 2023]

Prompt	Num tokens	Z-score	p-value
<p>...The watermark detection algorithm can be made public, enabling third parties (e.g., social media platforms) to run it themselves, or it can be kept private and run behind an API. We seek a watermark with the following properties:</p>			
<p><b>No watermark</b></p> <p>Extremely efficient on average term lengths and word frequencies on synthetic, microamount text (as little as 25 words)</p> <p>Very small and low-resource key/hash (e.g., 140 bits per key is sufficient for 99.999999999% of the Synthetic Internet)</p>	56	.31	.38
<p><b>With watermark</b></p> <ul style="list-style-type: none"> <li>- minimal marginal probability for a detection attempt.</li> <li>- Good speech frequency and energy rate reduction.</li> <li>- messages indiscernible to humans.</li> <li>- easy for humans to verify.</li> </ul>	36	7.4	6e-14

# Basic Watermarking with Green / Red Sampling

An original proposal from [Kirchenbauer et al., 2023]

## Sampling from a Random Subset of Words (soft take)

During generation, at each time step:

- 1 using  $w_{<t}$ , randomly split  $\mathcal{V}$  into  $\mathcal{V}(w_{<t}) \cup \mathcal{V}(w_{<t})$  of size  $\gamma|\mathcal{V}|, (1-\gamma)|\mathcal{V}|$
- 2  $Q_t(w | w_{<t}; \theta) \propto \exp \text{logit}(w, w_{<t}; \theta)$ ;
- 3  $Q_t(w | w_{<t}; \theta) \propto \exp \text{logit}(w, w_{<t}; \theta) + \delta$ ;
- 4 sample next word from  $Q_t(W | w_{<t}; \theta)$

Observing  $w_{[1:T]}$ :

- 1  $\forall t$ , compute  $\text{color}(w_t) \in \{\text{red}, \text{green}\}$
- 2 for watermarked texts:  $\mathbb{E}(n_{\text{green}}) \geq f(\gamma, T, \delta, S^*)$ , with  $S^*$  a measure of average surprisal
- 3 “excessively” green texts are artificial, “excessively” red texts are natural

- 🤖 - **generate** has parameters for  $1 - \gamma$  (`greenlist_ratio`) and  $\delta$  (`bias`), also `context_width` to control the context used in step 1.



## Part III

# Constrained Generation

# Constraining Text Generation

## Generating with simple constraints

- length (soft and hard) – for beam search
- no repetition (soft and hard penalties)
- with in-text / cross-text diversity (soft and hard penalties)

Updated search goals: **restricted search space** (hard constraints), **modified search objective** (soft)

# Constraining Text Generation

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- length (soft and hard) – for beam search
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Updated search goals: **restricted search space** (hard constraints), **modified search objective** (soft)

## A variety of constraints

- lexical choices (positive and negative, hard and soft) Keskar et al. [2019]
- language, idiom, sociolect (hard)
- style, consistency, toxicity, polarity, stance, etc (soft)
- optimizing other **global scores**: alignment score, backward model (translation); coverage score (summarization), etc.

# Guiding Decoding with Soft Constraints

## Soft constraints

A **soft or probabilistic constraint** for text  $w_{[1:T]}$  is a model  $P(A | w_{[1:T]}, \mathbf{C}; \lambda)$ , where  $A$  is a (binary) discrete attribute representing the constraint.

For instance:  $A = 1$  for harmful / toxic texts, 0 for harmless content;

Probabilistic constraints can be learned from supervision data:

- “**generatively**” with  $P(w_{[1:T]} | a, \mathbf{C}; \lambda) \forall a$  (learns / adapt multiple LMs - potentially costly)
- “**discriminatively**” with  $P(A | w_{[1:T]}, \mathbf{C}; \lambda)$  (LM + classification head)

Generative to discriminative score use Bayes rule

$$P(A | w_{[1:T]}, \mathbf{C}; \lambda) \propto P(A) P(w_{[1:T]} | A, \mathbf{C}; \lambda)$$

# Guiding Decoding with Soft Constraints

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## Decoding with constraints

A LM computes  $P(w_{[1:T]} | \boldsymbol{\theta})$ , how to generate  $w_{[1:T]}$  that simultaneously

- is fluent: high  $\log P(w_{[1:T]} | \mathbf{C}; \boldsymbol{\theta})$
- satisfies constraint with high  $F(w_{[1:T]}, \mathbf{C}) \propto \log P(A | w_{[1:T]}, \mathbf{C}; \boldsymbol{\lambda})$  ?

one requirement is based on the LM prior, one on the class posterior

# Guiding Decoding with Soft Constraints

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A **soft or probabilistic constraint** for text  $w_{[1:T]}$  is a model  $P(A | w_{[1:T]}, \mathbf{C}; \boldsymbol{\lambda})$ , where  $A$  is a (binary) discrete attribute representing the constraint.

For instance:  $A = 1$  for harmful / toxic texts, 0 for harmless content;

## Training-based methods

- fine-tuning, VAEs, GAN – all these methods requires retraining a model
- **[Ctrl]**, a class-conditional models (with class tokens) [Keskar et al., 2019].  
Learns  $\theta$  with  $[\text{ctrl:}]w_1 \dots w_T$ , a model for  $P(w_{[1:T]} | [\text{ctrl:}]; \theta)$ 
  - **[ctrl:]** is generic - represent style or domain or language or even length.
  - LLM needs to be trained with a finite set of predefined control codes
- **GeDi** [Krause et al., 2021] trains [ctrl] with  $\{a, \bar{a}\}$  and guide generation with **Bayes rule**

$$P(A = a | w_{[1:T]}; \boldsymbol{\lambda}) = \frac{P(a) \prod_t P(w_t | w_{<t}, a; \boldsymbol{\lambda})}{\sum_{a'} P(a') \prod_t P(w_t | w_{<t}, a'; \boldsymbol{\lambda})}$$

Soft constraint  $A$  is promoted in decoding with  $P(w | w_{<t}; \theta) P(a | w_{[1:t-1]}; \theta')^\alpha$

*The trick is to compute  $P(w_t | w_{<t}, A; \theta)$  **in parallel** for  $a, \bar{a}$*

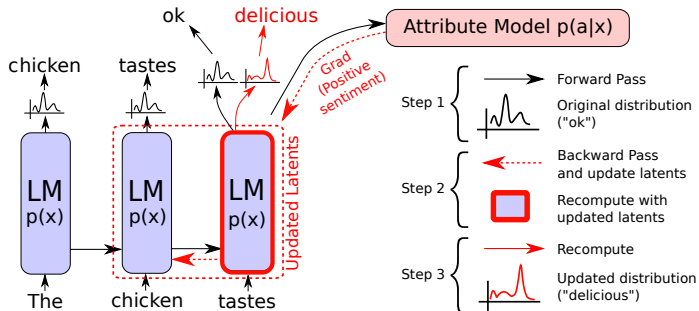
# A Plug-and-Play Method for Text Generation

The approach of [Dathathri et al., 2020]

## Gradient-based online adaptation

Sampling  $P(W_t | w_{<t}; \theta)$  depends on the logits at time  $t$ , which depend on the entire (Key,Value) store  $\mathbf{H}_{<t}$  at time  $t$ .

Main idea: adapt  $\mathbf{H}_t$  with  $\Delta \mathbf{H}_t$  to boost  $P(A | w_1 \dots w_t; \theta)$



# A Plug-and-Play Method for Text Generation

The approach of [Dathathri et al., 2020]

## Implementation

Iterate for 3-10 steps, starting with 0

$$\Delta \mathbf{H}_{<t} \leftarrow \Delta \mathbf{H}_{<t} + \alpha \frac{\nabla_{\Delta \mathbf{H}_{<t}} \log P(a | \mathbf{H}_{<t} + \Delta \mathbf{H}_{<t}; \boldsymbol{\lambda})}{\|\nabla_{\Delta \mathbf{H}_{<t}} \log P(a | \mathbf{H}_{<t} + \Delta \mathbf{H}_{<t}; \boldsymbol{\lambda})\|^\gamma}$$

Generate next token with  $\mathbf{H}_{<t} + \Delta \mathbf{H}_{<t}$



# A Plug-and-Play Method for Text Generation

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Generate next token with  $\mathbf{H}_{<t} + \Delta \mathbf{H}_{<t}$

## Caveats and Finesses

- $P(A | w_1 \dots w_t; \boldsymbol{\lambda})$  **must depend** on  $\mathbf{H}_{<t}$ : train via fine-tuning with the LM encoder.
- Regularize with additional KL-loss to remain close to  $P(W | w_{<t}; \boldsymbol{\theta})$
- Sample next word with a mixture of the original ( $\mathbf{H}_{<t}$ ) and adapted ( $\mathbf{H}_{<t} + \Delta \mathbf{H}_{<t}$ ) + meta parameters

# Generating with Rational Constraints

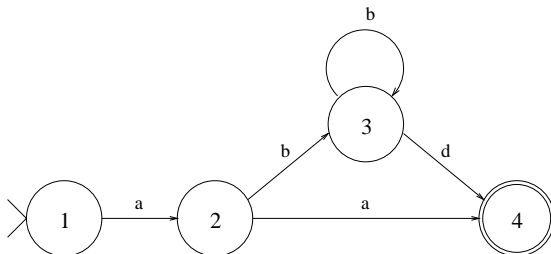
## Motivations for Hard Constraints

- 1 Watch your language 🤖 `bad_words_ids`
- 2 Force words in output (e.g QA): 🤖 `force_words_ids`
- 3 Question answering with fixed choices
- 4 Structured answers (e.g. JSON tables)
- 5 Code generation

# Generating with Rational Constraints

## Rational Languages

Rational languages are languages represented by Rational Expressions (a.k.a RegExps), are also languages represented by **(Deterministic) Finite Automata (DFAs)**.



Accomodate finite lists of words and sequences, numerics, http / mail addresses, etc

# Generating with Rational Constraints

## Implementing Rational Constraints

Requirements:

- 1 Transitions mapping (states, words) to next states.
  - restrict choice to valid continuations
  - apply transition; update state
- 2 List of final states: add `</s>` to valid word list

## Caveats

- 1 words are not tokens
- 2 compatible with beam ?
- 3 generalizes to simple (deterministic) CF grammars

Check it out - with outlines library: <https://github.com/dottxt-ai/outlines>

## Part IV

# Meta-Generation Strategies

# Meta-generation techniques

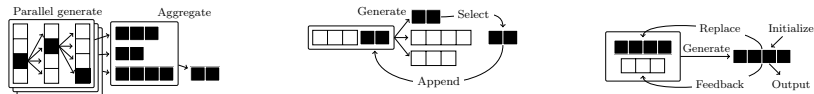


Figure from [Welleck et al., 2024]

## Meta-Generation Strategies

- Parallel search (combines multiple complete generations)
  - reranking (pick one in  $M$ )
  - transform (build a new one out of  $M$ )
- Heuristic step-level search (local search, MCTS,  $A^*$ )
- Refinement

# Reranking 101

## Main idea of reranking


### Reranking as Meta Generation

- 1 **generate**  $M$  solutions  $\mathcal{W}_S = \{[w^{(m)}]_{[1:T]}, m = 1 \dots M\}$  based on model  $\log P([w^m]_{[1:T]} | \mathbf{C}; \boldsymbol{\theta})$
- 2 **evaluate**  $[w^{(m)}]_{[1:T]}$  with alternative, global score  $F([w]_{[1:T]}], \mathbf{C}', \boldsymbol{\theta}')$
- 3 **return**  $\operatorname{argmin}_m F([w^{(m)}]_{[1:T]}], \mathbf{C}', \boldsymbol{\theta}')$

# Reranking 101

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  - 3 **return**  $\operatorname{argmin}_m F([w^{(m)}]_{[1:T]}, \mathbf{C}', \boldsymbol{\theta}')$
- Design of **generate** (for  $M$ ): (diverse) beam-search ? (diverse) sampling ? stochastic beam search ? Multiple models and checkpoints ? Multiple prompts? Impact of  $M$ ?  
 `num_return_sequences`
  - Design of **evaluate**: length control; score of a larger or better model ( $\boldsymbol{\theta}'$ ); increased context ( $\mathbf{C}'$ ); use auxiliary models of grammaticality, style, toxicity, stance, polarity; use result of execution (code); also watermarking; confidentiality; etc.



# Minimum Bayes Risk Decoding

## Context and Concepts

$\ell([w_{1:T}], [v_{1:S}]) : (<s>\mathcal{V}^*</s>) \times (<s>\mathcal{V}^*</s>) \rightarrow \mathbb{R}$  a **global dissimilarity function**  
 $\ell$  is small when two solutions are similar

- $\ell([w_{1:T}], [v_{1:S}]) = 1 - \mathbb{I}([w_{1:T}] = [v_{1:S}])$   
**one-hot dissimilarity**, all (non identical) pairs of sequences have  $\ell = 1$
- $\ell([w_{1:T}], [v_{1:S}]) = 1 - \text{NED}([w_{1:T}], [v_{1:S}])$   
**Normalized Edit Distance**, normalized minimum number of edits from  $w_{1:T}$  to  $v_{1:S}$
- $\ell([w_{1:T}], [v_{1:S}]) = 1 - \text{BLEU}([w_{1:T}], [v_{1:S}])$   
**reference based metrics - n-gram overlap** (BLEU, METEOR for MT, Rouge for summarization)
- $\ell([w_{1:T}], [v_{1:S}]) = -\cos(\text{Emb}([w_{1:T}]), \text{Emb}([v_{1:S}]))$   
**cosine dissimilarity** in embedding space, generalize to neural metrics (COMET, BLEURT, BertScore)  
 [Suzgun et al., 2023]

# Minimum Bayes Risk Decoding

## Main idea

For fixed  $[w_{1:t}]$ , the risk of  $[w_{1:T}]$

$$\begin{aligned} R([w_{1:T}]) &= \mathbb{E}_{v_{[1:S]} \sim P}(\ell([w_{1:T}], v_{[1:S]})) \\ &= \sum_{v_{[1:S]}} P(v_{[1:S]}) \ell([w_{1:T}], v_{[1:S]}) \end{aligned}$$

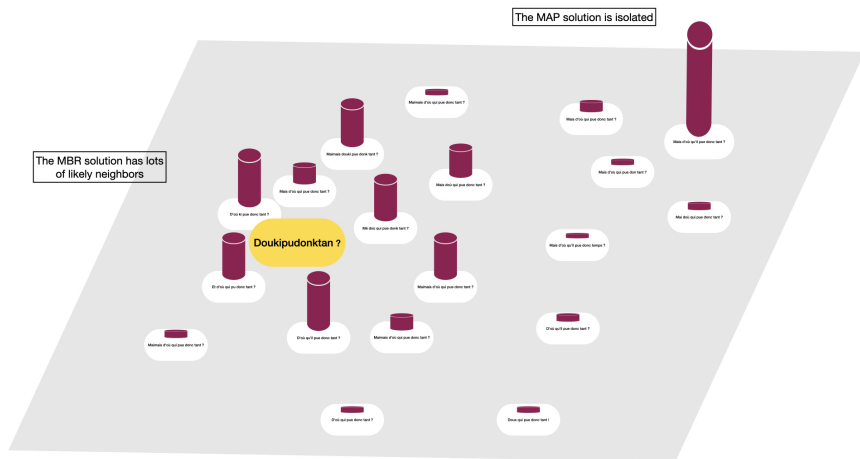
Minimum Bayes Risk decoding seeks

$$\begin{aligned} w_{[1:T^*]}^* &= \operatorname{argmin}_{T, [w_{1:T}]} R([w_{1:T}]) \\ &= \operatorname{argmin}_{T, [w_{1:T}]} \mathbb{E}_{S, v_{[1:S]} \sim P}(\ell([w_{1:T}], v_{[1:S]})) \\ &= \operatorname{argmin}_{T, [w_{1:T}]} \sum_{S, v_{[1:S]}} P(v_{[1:S]}) \ell([w_{1:T}], v_{[1:S]}) \end{aligned}$$

The best sequence is (on average) the closest to all other sequences

## Minimum Bayes Risk Decoding

Intuition: why is MBR is a good idea ?



# Minimum Bayes Risk Decoding

Intuition: why is MBR is a good idea ?

0- the mode ( $\text{argmax } P([w_{1:T}] | \theta)$ ) may be *anomalous and risky* [Eikema and Aziz, 2020]

1- If likely solutions (high  $P([w_{1:T}] | \theta)$ ) have a good quality, being close to many good solutions ( $[w_{1:T}^*]$ ) is also likely to have a good quality [smoothness of search space]

2- For the one-hot dissimilarity:  $\ell([w_{1:T}], [v_{1:S}]) = 1 - \mathbb{I}([w_{1:T}] = [v_{1:S}])$ ,

$$\begin{aligned} \mathbb{E}_{[v_{1:S}] \sim P}(\ell([w_{1:T}], [v_{1:S}])) &= \sum_{[v_{1:S}] \neq [w_{1:T}]} P([v_{1:S}] | \theta) \\ &= 1 - P([w_{1:T}] | \theta) \end{aligned}$$

Minimizing the risk maximizes the model probability: *back to MAP !*

3- The MAP maximizes a proxy quality score  $P(w_{1:t} | \theta)$ , MBR directly optimizes the true metric  $\ell()$  instead

See also the motivations of Bertsch et al. [2023].

# Minimum Bayes Risk Decoding

## Theory and Practice of MBR

### Two sources of intractability

$$w_{[1:t]}^* = \underset{T, w_{[1:t]}}{\operatorname{argmin}} \sum_{s, v_{[1:s]}} P(v_{[1:s]}) \ell([w_{[1:T]}], [v_{[1:s]}])$$

- ①  $\underset{T, w_{[1:T]}}{\operatorname{argmin}}$ : argmin in a very very large set
- ②  $\sum_{s, v_{[1:s]}}$ :  $\sum$  over many many terms

# Minimum Bayes Risk Decoding

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- ②  $\sum_{s, [v_{[1:s]}]}$ :  $\sum$  over many many terms

### Two practical remedies

- ① argmin in a very very large set  $\Rightarrow$  restrict search to  $\mathcal{W}_s$
- ②  $\sum$  over many many terms  $\Rightarrow$  replace  $\mathbb{E}()$  by Monte-Carlo approximation of size  $|\mathcal{W}_{MC}|$

$$w_{[1:t]}^* = \underset{T, [w_{[1:T]}] \in \mathcal{W}_s}{\operatorname{argmin}} \sum_{[v_{[1:s]}] \in \mathcal{W}_{MC}} \ell([w_{[1:T]}], [v_{[1:S]}])$$

# Minimum Bayes Risk Decoding

MBR: a meta-generation algorithm

$\ell()$ : Comparator function, model  $P(\cdot | C; \theta)$

```

1:  $\mathcal{W}_{MC} \leftarrow \text{generate}(P(\cdot | C; \theta), N, \dots)$ 
2:  $\mathcal{W}_S \leftarrow \text{generate}(P(\cdot | C; \theta), M, \dots)$ 
3:  $mins \leftarrow +\infty$ 
4: for  $[w_{1:T}] \in \mathcal{W}_S$  do
5:    $s \leftarrow 0, mbr \leftarrow \langle s \rangle \langle /s \rangle$ 
6:   for  $[v_{1:S}] \in \mathcal{W}_{MC}$  do
7:      $s \leftarrow s + \ell([w_{1:T}], [v_{1:S}])$ 
8:   end for
9:   if  $s < mins$  then
10:     $mins \leftarrow s, mbr \leftarrow [w_{1:T}]$ 
11:   end if
12: end for
```

- **generate 1:** is for MC estimates: **prefer sampling with replacement**, unbiased (ancestral)
- **generate 2:** is to identify promising solutions: **prefer beam-search**, if possible diverse
- Alternative for  $\mathcal{W}_S$ : reuse  $\mathcal{W}_{MC}$  - back to reranking
- Alternative for  $\mathcal{W}_S$ : use multiple models, multiple checkpoints, multiple prompts, etc.
- Run-time is Sampling time +  $O(MN)$ ; larger  $N$  yields better MC estimates; larger  $M$  explores a larger search space

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# Better Searching for Good Solutions with MCTS

Monte-Carlo Tree Search is by [Kocsis and Szepesvári, 2006]

The problem with global scores  $F([w_{1:T}], C)$

- Searching with  $P([w_{1:T}] | \mathbf{C}; \theta)$  may yield poor / inappropriate solutions
- Ensemble-based methods (n-best reranking, MBR) require multiple inferences, no guarantee of improvements

**MCTS delivers solutions with a high global score, based on estimates of  $F([w_{1:T}], C)$  for partial sequences  $w_{1:t}$ .**

# Better Searching for Good Solutions with MCTS

Monte-Carlo Tree Search is by [Kocsis and Szepesvári, 2006]

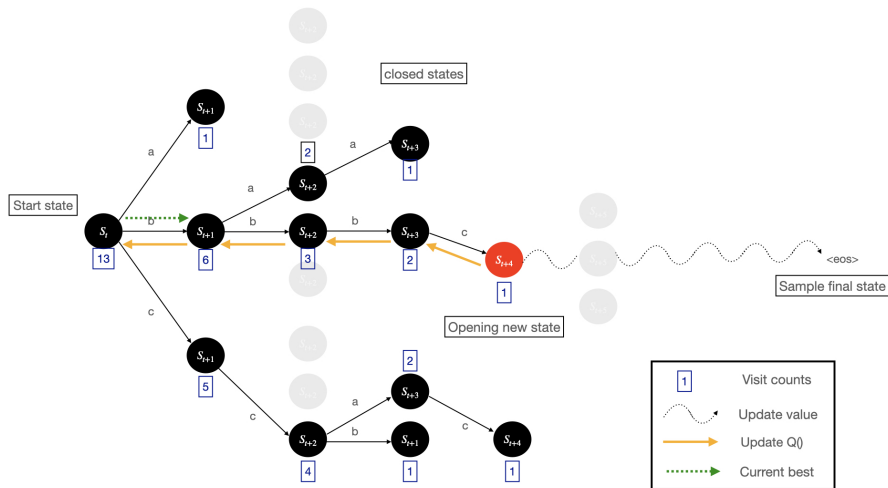
## Concept and Terminology (adapted from RL / POMDP)

- **State:**  $S_t \Leftrightarrow$  context + current prefix  $C, w_{[1:t]}$ ;  $\mathcal{S}$  is the set of states (prefixes).  
States can be **complete** ( $w_T = </s>$ ) or **uncomplete**.
- **Actions:** pick next possible token  $w_{t+1} \in \mathcal{V}$
- **Using action  $w$  in state  $S_t$ :** yields new state  $S_t \oplus w \equiv w_{[1:t+1]} = w_{[1:t]}w$
- **Policy  $\pi_\theta$ :**  $\mathcal{S} \rightarrow \mathcal{V}$ ; next action selection rule. For instance:
  - $\pi_\theta(S_t) = \operatorname{argmax}_w P(w|S_t; \theta)$ : **greedy** policy (deterministic)
  - $\pi_\theta(S_t) = w \sim P(w|S_t; \theta)$ : **sampling** policy (non-deterministic) - also top- $k$ , top- $p$  etc.
- **Value** (of a state, given policy):  $v_\pi : \mathcal{S} \rightarrow \mathbb{R}$ ;  $v_\pi(S_t)$  estimates **the best score  $F()$  attainable from  $S_t$** .

Use state values to obtain MC samples of local subtrees that guide the generation policy towards leaf nodes with large scores.

# Better Searching for Good Solutions with MCTS

Monte-Carlo Tree Search is by [Kocsis and Szepesvári, 2006]



## Generating one token with MCTS

# Better Searching for Good Solutions with MCTS

Monte-Carlo Tree Search is by [Kocsis and Szepesvári, 2006]

```

1: procedure MCTS( $K : \text{int}$ )
2:    $S \leftarrow S_0 (\equiv C, \langle s \rangle)$ 
3:   while !complete( $S$ ) do
4:     for  $K$  iterations do
5:       MCTS-Explore( $S$ )
6:     end for
7:      $w^* \leftarrow \operatorname{argmax}_{w \in \mathcal{V}} \text{cnt}(S \oplus w)$ 
8:      $S \leftarrow S \oplus w^*$ 
9:   end while
10:  return  $S$ 
11: end procedure

1: procedure PUCT-SCORE( $S, w$ )
2:    $U \leftarrow Q(S \oplus w)$ 
3:    $U \leftarrow U + c_{\text{puct}} P(w | S; \theta) \frac{\sqrt{\text{cnt}(S)}}{1 + \text{cnt}(S, w)}$ 
4:   return  $U$ 
5: end procedure

```

```

1: procedure MCTS-EXPLORE( $S : \text{state}$ )
2:    $\text{cnt}(S) \leftarrow \text{cnt}(S) + 1$ 
3:    $w^* \leftarrow \operatorname{argmax}_w \text{UCT-Score}(S, w)$ 
4:   if open( $S \oplus w^*$ ) ^ !complete( $S \oplus w^*$ ) then
5:      $Q \leftarrow \text{MCTS-Explore}(S \oplus w^*)$ 
6:      $Q(S) \leftarrow \max(Q(S), Q)$ 
7:   else if !complete( $S$ ) then
8:     open( $S$ )  $\leftarrow$  true
9:      $\triangleright$  aggregate with max or avg
10:     $Q \leftarrow \operatorname{argmax}_{\text{open}(S \oplus w)} v_{\pi}(S \oplus w)$ 
11:   else
12:      $Q \leftarrow F(S)$ 
13:   end if
14:   return  $Q$ 
15: end procedure

```

PUCT-SCORE trades-off high scores ( $Q$ ) and likely, unvisited states

# Better Searching for Good Solutions with MCTS

Monte-Carlo Tree Search is by [Kocsis and Szepesvári, 2006]

## Computing state values

In state  $S$ , how to estimate  $v_\pi(S)$ ?

- 1 **Sampling based**: apply sampling using **roll-out** policy  $P(\cdot | S; \theta)$  (e.g. [Chaffin et al., 2022]) return underestimates, as costly as a complete generation for each simulation.
- 2 **Learning based**: learns to predict  $v_\pi(S; \lambda)$  using an auxiliary network [Leblond et al., 2021] get complete (complete) samples  $[w_{1:T}]$  and associated scores; learns to predict scores for **incomplete states**; this can be hard.
- 3 **Repurpose** value networks trained with **reinforcement learning** (PPO) during LLM **alignment step** [Liu et al., 2024] show improvements even when using PPO-tuned language models.

# Generating Texts Non-Auto-Regressively

## Parallel Text Generation

Standard left-to-right / right-to-left decoding is slow

Decoding in arbitrary order does not solve this [Welleck et al., 2019]

Alternative: generate multiple words simultaneously

How ? **Parallel Unmasking**.

# Generating Texts Non-Auto-Regressionly

Mask-Predict by Ghazvininejad et al. [2019]

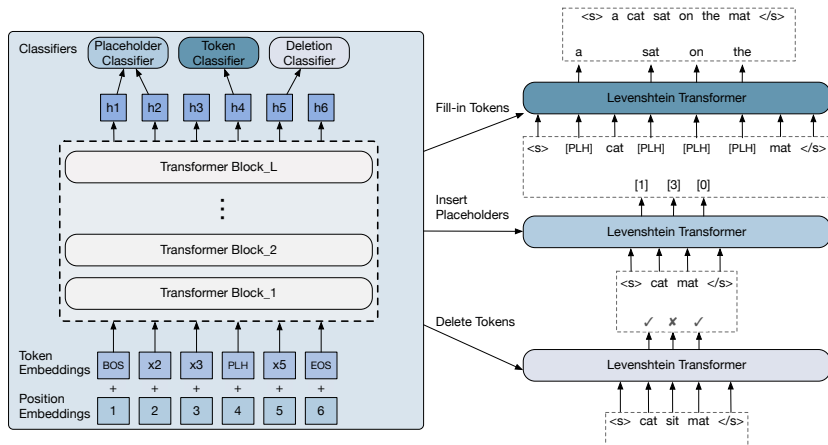
```

1: procedure MASK-PREDICT
  Input:  $\mathbf{C}$  : Context,  $T$ : Target Length
  Output: Generated Sequence
2:    $\forall t \in [1 : T], w_t \sim \text{Unif}(\mathcal{V})$ 
3:   for  $K$  iterations do
4:     ToMask  $\leftarrow$  top- $k_t(-\log P(w_t | \mathbf{C}, w_{-t}; \theta))$ 
5:     for  $(t \in \text{ToMask})$  do
6:        $w_t \leftarrow \text{MASK}$ 
7:     end for
8:     for  $(t \in \text{ToMask})$  do
9:        $w_t \leftarrow \text{unmask}(w_t)$ 
10:    end for
11:  end for
12: end procedure

```

- a better initialization samples independently given  $\mathbf{C}$
- **unmask**( $l_9$ ) can be argmax or obtained via sampling
- $T$  is unknown ? Generate with **multiple lengths** in parallel
- masking and generation can be performed in parallel
- **$K$  and  $k$  trade-offs** speed and fluency
- **recover Gibbs sampling** with  $k = 1$  and iterative masking (instead of top- $k$ )

# Generating Texts Non-Auto-Regressively

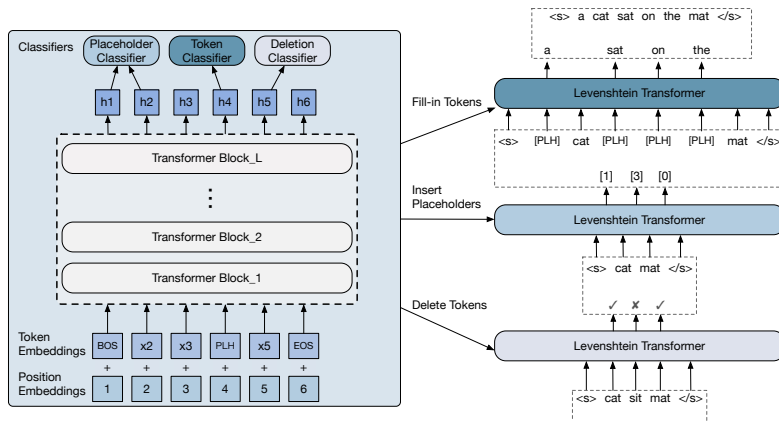


The Levenshtein Transformer [Gu et al., 2019]

- “Multimodality” problem and solutions (latent alignments, KD, etc) [Xiao et al., 2023]
- Mostly used for standard translation tasks (also: term constraints [Xu and Carpuat, 2021])
- Decoding starts from scratch or initial solution [Xu et al., 2023]



# Generating Texts Non-Auto-Regressively



LevT uses

3 classifiers to predict Deletions and Insertions

**D** **deletion** classifier predicts  $y \in \{0, 1\}$

**I** **placeholder** classifier predicts  $y \in [0 : N]$

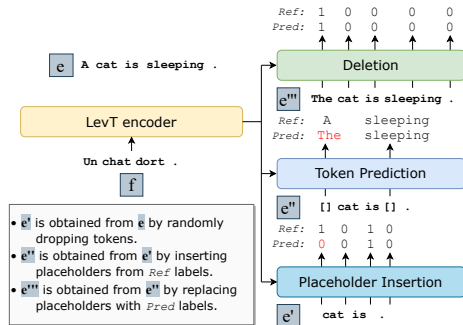
**I** **token** classifier predicts  $y \in [1 : |V|]$

# Generating Texts Non-Auto-Regressively

## Training with parallel sentences (f, e)

- 1 erase random words in e, yields t''
- 2 train placeholder & token prediction with samples (t'', e), (t'', e)
- 3 generate output e
- 4 train deletion prediction with (e, e)

**Decode** with  $t' = \langle s \rangle \langle /s \rangle$ : PLH - TOK - DEL  
 + **repeat in iterative refinement**



## Dual Policy learning with:

- **roll-in policy**  $\pi_{ins}$  for [I]nsertion: empty string or random deletion from **e**
- **roll-in policy**  $\pi_{del}$  for [D]eletion: model's Insertions
- **expert policy**  $\pi^*$  from the optimal alignment  $\Leftrightarrow$  **Edit Distance**

**An effective model for NAR Machine Translation**

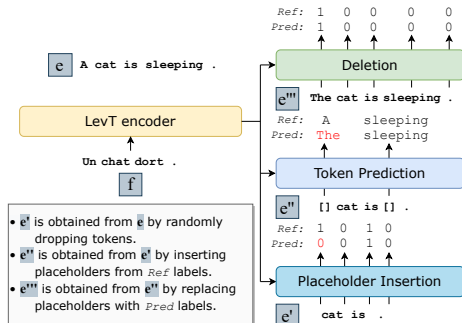
# Generating Texts Non-Auto-Regressively

## Training with parallel sentences (f, e)

- 1 erase random words in e, yields  $t'$
- 2 train placeholder & token prediction with samples ( $t'$ , e), ( $t''$ , e)
- 3 generate output e
- 4 train deletion prediction with (e, e)

Decode with  $t' = \langle s \rangle \langle /s \rangle$ : PLH - TOK - DEL

+ repeat in iterative refinement



## Dual Policy learning with:

- roll-in policy  $\pi_{ins}$  for [I]nsertion: empty string or random deletion from  $e$
- roll-in policy  $\pi_{del}$  for [D]eletion: model's Insertions
- expert policy  $\pi^*$  from the optimal alignment  $\Leftrightarrow$  Edit Distance

# Refinement

# Conclusions

## Generation is Tricky

- Training procedures matter
- Generation parameter matter - both for speed and quality
- There is more than top- $k$  and top- $p$

## Generation is not Solved

- Generation with refinement and self-critics
- Multi-hop / text generation and planing

# Conclusions

## Generation is Tricky

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# Part V

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