A statistical framework of watermarks for large language models:

Pivot, detection efficiency and optimal rules

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Outline

Introduction

A statistical framework for watermark detection

Efficiency measure and optimal detection rule

Application to Gumbel-max watermark

Application to inverse transform watermark

Summary

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A statistical framework for watermark detection

Efficiency measure and optimal detection rule

Application to Gumbel-max watermark

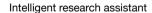
Application to inverse transform watermark

Summary

Large language models (LLMs)

- LLMs is advanced AI systems trained to understand and generate human-like text.
- ► Many applications: content creation, customer service, education, code generation, healthcare, business intelligence,







Automated document generation and editing

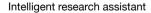


Creative content creation

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Creative content creation

► However, there are some issues......

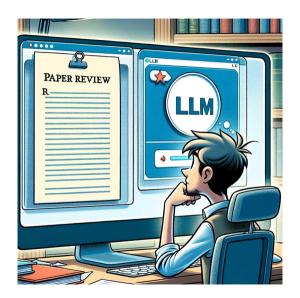
Academic integrity

Did the student write this homework/paper by himself, or did an LLM lend a hand?



Peer review or LLM review?

- ▶ Liang et al. [2024] finds that between 6.5% and 16.9% reviews of some ML conferences were substantially modified by LLMs.
- Is your paper review really your own, or did an LLM lend a hand?



Document authenticity

▶ Is an impressively detailed patient report written by the patient or an LLM?



Central problem

Given a text, how to determine whether it is generated by an LLM.

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- ▶ Directly comparing the distribution of LLM outputs and human-written texts are neither accurate nor reliable [Weber-Wulff et al., 2023] and often biased [Krishna et al., 2024, Sadasivan et al., 2023, Liang et al., 2023].

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- ► More accurate detection requires us to have inner access of LLMs and thereby transition from a black-box to a white-box approach.
- Watermark is such an elegant and powerful method.

Watermark

- ► Watermarking enables more accurate detection of LLM-generated text by injecting subtle statistical patterns during text generation.
- ► Those patterns are unlikely to be replicated by a human but are constantly repeated by the watermarked LLM.
- ▶ Detecting the patterns help us detect the watermarks or equivalently the LLM-generated texts.

Preliminaries about LLM watermarks

Tokenization

- ▶ The tokenization process breaks down the text into smaller units called "tokens."
- ► Tokens can be words, parts of words, or even punctuation marks.¹

GPT-3.5 & GPT-4 GPT-3 (Legacy)

OpenAI's large language models (sometimes referred to as GPTs) process text using tokens, which are common sequences of characters found in a set of text. The models learn to understand the statistical relationships between these tokens and excel at producing the next token in a sequence of tokens.

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Tokens Characters 57 299

[5109, 15836, 596, 3544, 4221, 4211, 320, 57753, 14183, 311, 439, 480, 2898, 82, 8, 1920, 1495, 1701, 11460, 11, 902, 527, 4279, 24630, 315, 5885, 1766, 304, 264, 743, 315, 1495, 13, 578, 4211, 4048, 311, 3619, 279, 29564, 12135, 1990, 1521, 11460, 323, 25555, 520, 17843, 279, 1828, 4037, 304, 264, 8668, 315, 11460, 13]

¹Refer to the website https://platform.openai.com/tokenizer for more examples of tokenization.

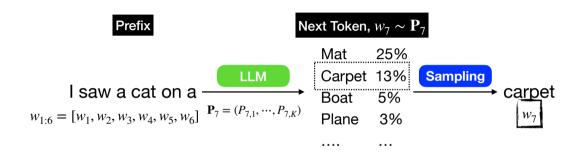
Let $W = \{1, 2, ..., K\}$ be the vocabulary and w a token therein.

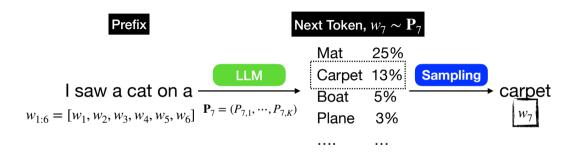
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- ▶ The vocabulary size $K = |\mathcal{W}|$ is large and varies for difference models.
- K = 50272 for the OPT-1.3B model; = 32000 for the LLaMA-7B model.

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- ▶ The vocabulary size $K = |\mathcal{W}|$ is large and varies for difference models.
- κ K = 50272 for the OPT-1.3B model; = 32000 for the LLaMA-7B model.
- An LLM \mathcal{M} generates each token sequentially by sampling from a probability distribution conditioned on previous tokens:

$$w_t \sim m{P}_t$$
 where $m{P}_t = \mathcal{M}(w_{1:(t-1)})$ is a distribution on \mathcal{W} .

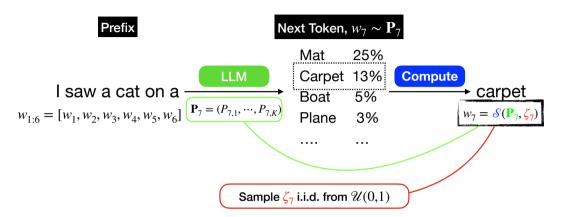
▶ The categorical distribution P_t is referred to next-token prediction (NTP) distribution.



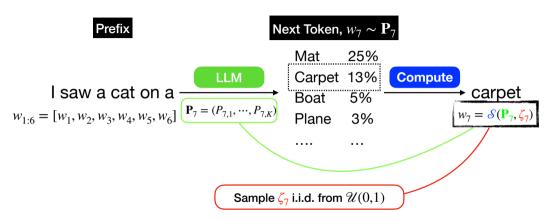


Watermarks are embedded in each next-token sampling.

Watermarked generation



Watermarked generation



- S is referred to as decoder.
- ▶ The watermark signal is the dependence of w_7 on ζ_7 .

A baby watermark

- ▶ Let $W = \{0, 1\}, P_t = (P_{t,0}, P_{t,1}), \zeta_t$ be i.i.d. copies of U(0, 1).
- ► The decoder is

$$w_t = \mathcal{S}(\boldsymbol{P}_t, \zeta_t) = egin{cases} 0 & ext{ if } \zeta_t \leq P_{t,0} \ 1 & ext{ otherwise.} \end{cases}$$

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▶ This watermark is unbiased in the following sense:

Definition (Unbiased)

For any
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 and $w\in\{0,1\}$,

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- ▶ If ζ_t is large, then w_t is more likely to be 1 instead of 0, and vice versa.
- Using the following statistic for detecting the watermark:

$$\sum_{t=1}^{n} (2w_t - 1)(2\xi_t - 1).$$

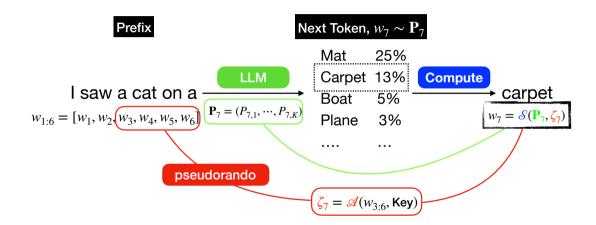
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- **Q1** How to make these $\zeta_{1:n}$ recoverable?
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Q1. Use pseudorandom variables



Hash function A

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Q1. Decoder $\mathcal{S}^{\mathrm{gum}}$ from Gumbel-max trick

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Gumbel-max trick [Gumbel, 1948]

Let $\Xi = [0,1]^K$ and $\zeta = (U_1, U_2, \dots U_K) \in \Xi$ with U_k 's i.i.d. copies of $\mathcal{U}(0,1)$. The Gumbel-max trick asserts that

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Gumbel-max watermark [Aaronson, 2023]

$$\mathcal{S}^{\mathrm{gum}}(\boldsymbol{P},\zeta) = \arg\max_{k \in [K]} \left\{ \frac{1}{P_k} \cdot \log U_k \right\} \quad \text{where} \quad \zeta = (U_1,\ldots,U_K).$$

Q1. Decoder S^{inv} from inverse transform sampling

Inverse transform sampling

The CDF of \boldsymbol{P} on \mathcal{W} is

$$F_{\mathbf{P}}(x) = \sum_{w' \in \mathcal{W}} P_{w'} \cdot \mathbf{1}_{\{w' \le x\}}.$$

Taking as input $U \sim U(0,1)$, the generalized inverse of this CDF is defined as

$$F_{\mathbf{P}}^{-1}(U) = \min \left\{ x : F_{\mathbf{P}}(x) \ge U \right\}.$$

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Inverse transform watermark [Kuditipudi et al., 2023]

$$\mathcal{S}_{\mathrm{inv}}(\boldsymbol{P},\zeta) := \pi \circ (F_{\pi(\boldsymbol{P})}^{-1}(U))$$
 where $\zeta = (U,\pi), \ U \sim \mathcal{U}(\Pi), \ U \perp \pi.$

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A statistical framework is needed.

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Review

Two-step watermarked generation

- **1.** Generate a pseudorandom number: $\zeta_t = \mathcal{A}(w_{1:(t-1)}, \text{Key}) \sim \mathcal{U}(\Xi)$.
- **2.** Compute the next token: $w_t = \mathcal{S}(\mathbf{P}_t, \zeta_t)$.

Definition (Watermark)

A watermark is defined by a tuple (S, A, Key).

The watermark signal is the dependence of each w_t on ζ_t .

Definition (Unbiased)

We say the decoder S is unbiased if for any P and $w \in W$,

$$\mathbb{P}_{\zeta \sim \mathcal{U}(\Xi)}(\mathcal{S}(\boldsymbol{P},\zeta) = w) = P_w.$$

Given data $(w_{1:n}, \zeta_{1:n})$,

 $H_0: w_{1:n}$ is written by human, versus $H_1: w_{1:n}$ is watermarked by $(\mathcal{S}, \mathcal{A}, \text{Key})$.

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Working Hypothesis

- ▶ Under H_0 , $(w_t, \zeta_t) \mid (w_{1:(t-1)}, \zeta_{1:(t-1)}) \stackrel{d}{=} P_{\mathsf{human},t} \times \mathcal{U}(\Xi)$.
- ▶ Under H_1 , $(w_t, \zeta_t) \mid (w_{1:(t-1)}, \zeta_{1:(t-1)}) \stackrel{d}{=} (\mathcal{S}(\zeta_t, \mathbf{P}_t), \zeta_t)$ and $\zeta_t \sim \mathcal{U}(\Xi)$.

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But, we don't know $P_{human,1}, \ldots, P_{human,n}$ and other P_1, \ldots, P_n .

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But, we don't know $P_{human,1}, \ldots, P_{human,n}$ and other P_1, \ldots, P_n .

Impossible to estimate these unknown P_t 's.

Detection: The solution

Find a pivotal statistic $Y_t = Y(w_t, \zeta_t)$ such that

- ▶ Under H_0 , $Y_t \sim \mu_0$ regardless of $P_{\text{human},t}$.
- ▶ Under H_1 , $Y_t \sim Y(S(\zeta_t, P_t), \zeta_t)$. Hence, $Y_t | P_t \sim \mu_{1,P_t}$.

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Finall formulation

$$H_0: Y_t \overset{i.i.d.}{\sim} \mu_0 \ \forall t \in [n]$$
 versus $H_1: Y_t | \mathbf{P}_t \sim \mu_{1,\mathbf{P}_t} \ \forall t \in [n].$

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▶ A score function $h : \mathbb{R} \to \mathbb{R}$ introduces a detection rule $T_h = \sum_{t=1}^n h(Y_t)$ which reject H_0 if T_h is larger than a threshold.

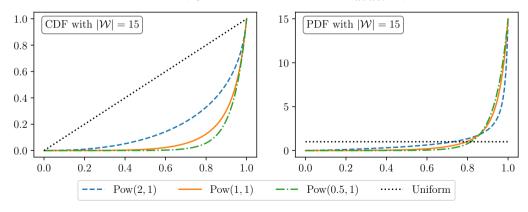
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Let's see some detection examples.

- ▶ Recall $S^{\text{gum}}(\mathbf{P}, \zeta) = \arg\max_{k \in [K]} \frac{\log U_k}{P_k}$ and $\zeta_t = (U_{t,1}, \dots, U_{t,K}) \in [0, 1]^K$.
- ▶ The pivotal statistic is $Y_t^{ars} = U_{t,w_t}$.

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- ▶ The pivotal statistic is $Y_t^{ars} = U_{t,w_t}$.
- ▶ Under H_0 , $Y_t^{\text{ars}} \stackrel{i.i.d.}{\sim} \mu_0 = \mathcal{U}(0,1)$.
- ▶ Under H_1 , the CDF of μ_{1,P_t} is $\mathbb{P}_1(Y_t^{ars} \leq y | P_t) = \sum_{k \in [K]} P_{t,k} y^{1/P_{t,k}}$.

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Default detection for Gumbel-max watermark [Aaronson, 2023]

Aaronson proposes to reject H_0 if the following quantity is larger than a given threshold:

$$T_{h_{\mathrm{ars}}} = \sum_{t=1}^{n} h_{\mathrm{ars}}(Y_t^{\mathrm{ars}})$$
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- ▶ Under H_0 , $h_{ars}(Y_t^{ars}) \stackrel{i.i.d.}{\sim} Exp(1)$ so that $\mathbb{E}_0 T_{ars} = n$.
- ▶ Under H_1 , $\mathbb{E}_1 T_{ars} \ge n + \left(\frac{\pi^2}{6} 1\right) \sum_{t=1}^n \mathbb{E}_1 \mathrm{Ent}(\boldsymbol{P}_t)$ where $\mathrm{Ent}(\boldsymbol{P}_t)$ is Shannon entropy defined by $\sum_{k=1}^K P_{t,k} \log \frac{1}{P_{t,k}}$.

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- ▶ Under H_1 , $\mathbb{E}_1 T_{\text{ars}} \ge n + \left(\frac{\pi^2}{6} 1\right) \sum_{t=1}^n \mathbb{E}_1 \text{Ent}(\boldsymbol{P}_t)$ where $\text{Ent}(\boldsymbol{P}_t)$ is Shannon entropy defined by $\sum_{k=1}^K P_{t,k} \log \frac{1}{P_{t,k}}$.
- Other h? Using the same Y_t^{ars} , Fernandez et al. [2023] finds that $-\log(1-y)$ works better than the variant $\log y$.

Detection for inverse transform watermark

- ▶ Recall that $\zeta_t = (\pi_t, U_t) \in \Pi \times [0, 1]$. Define $\eta(k) = (k-1)/(K-1)$.
- ▶ The pivotal statistic used by Kuditipudi et al. [2023] is $Y_t^{\text{dif}} = |U_t \eta(\pi_t(w_t))|$.

Detection for inverse transform watermark

- ▶ Recall that $\zeta_t = (\pi_t, U_t) \in \Pi \times [0, 1]$. Define $\eta(k) = (k-1)/(K-1)$.
- ▶ The pivotal statistic used by Kuditipudi et al. [2023] is $Y_t^{\text{dif}} = |U_t \eta(\pi_t(w_t))|$.

Default detection for inverse transform watermark [Kuditipudi et al., 2023]

Kuditipudi proposes to reject H_0 if the following quantity is larger than a given threshold:

$$\mathcal{T}_{h_{\mathrm{neg}}} = \sum_{t=1}^n h_{\mathrm{neg}}(Y_t^{\mathrm{dif}})$$
 where $h_{\mathrm{neg}}(y) = -y$.

- Y_t^{dif} should be smaller under H_1 than under H_0 due to the correlation between U_t and $\eta(\pi_t(w_t))$.
- ▶ No analysis for μ_0 and μ_{1,P_t} as well as the detection rationale.

Questions studied

- ▶ Multiple detection rules for Gumbel-max watermark. No theoretical justification.
- No theoretical analysis for the inverse transform watermark.
- ▶ What is the "optimal" score function *h*?

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- No theoretical analysis for the inverse transform watermark.
- ▶ What is the "optimal" score function *h*?

Main questions

- Could we propose an efficiency measure to rank different detection rule?
- ▶ Could we find the optimal detection rule according to the efficiency measure?

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$$H_0: Y_t \overset{i.i.d.}{\sim} \mu_0 \ \forall t \in [n]$$
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- ▶ Under H_0 , $Y_t \stackrel{i.i.d.}{\sim} \mu_0$ so that Type I error can be controlled.
- ▶ Under H_1 , $Y_t | P_t \sim \mu_{1,P_t}$. Unknown and varies P_t 's make analysis hard.

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Key idea

Given a prior set \mathcal{P} , we consider the least-favorable type II error over \mathcal{P} .

• We then believe all the LLM-generated P_t 's fall into P.

Theorem

Fix a pivot scalar Y and a score function h. Let the Type I error of T_h be α . Then

$$\lim \sup_{n \to \infty} \sup_{\forall P_t \in \mathcal{P}} [1 - \mathbb{E}_1 T_h(Y_{1:n})]^{1/n} \le \exp(-R_{\mathcal{P}}(h)),$$

where $R_{\mathcal{P}}(h)$ is \mathcal{P} -dependent efficiency rate defined by

$$R_{\mathcal{P}}(h) = -\inf_{\theta \geq 0} \left\{ \theta \mathbb{E}_0 h(Y) + \log \phi_{\mathcal{P},h}(\theta) \right\} \quad \text{with} \quad \phi_{\mathcal{P},h}(\theta) = \sup_{\boldsymbol{P} \in \mathcal{P}} \mathbb{E}_1[e^{-\theta h(Y)} | \boldsymbol{P}].$$

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- Motivated by large deviation theory.
- ▶ $R_{\mathcal{P}}(h) \ge 0$ by definition.
- ▶ The upper bound is tight under some regularities.

Optimal detection rule

ightharpoonup Maximize to find the optimal score function h^* :

$$h^* = \arg \max_h R_{\mathcal{P}}(h)$$

where we need to solve the following minimax problem:

$$\inf_{h} \left\{ \mathbb{E}_{0}h(Y) + \sup_{\boldsymbol{P} \in \mathcal{P}} \log \left(\mathbb{E}_{1}[e^{-h(Y)}|\boldsymbol{P}] \right) \right\}.$$

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▶ It is generally not jointly convex-concave.

How to maximize $R_{\mathcal{P}}(h)$

$$\inf_{h} \left\{ \mathbb{E}_{0}h(Y) + \sup_{\boldsymbol{P} \in \mathcal{P}} \log \left(\mathbb{E}_{1}[e^{-h(Y)}|\boldsymbol{P}] \right) \right\}$$

Theorem

If there exists an $\mathbf{P}^{\star} \in \mathcal{P}$ and a score function class \mathcal{H} such that for all $h \in \mathcal{H}$,

$$\sup_{\boldsymbol{P}\in\mathcal{P}}\mathbb{E}_1[e^{-h(Y)}|\boldsymbol{P}] = \mathbb{E}_1[e^{-h(Y)}|\boldsymbol{P}^{\star}], \tag{\boldsymbol{P}^{\star}}$$

$$h^* := \log \frac{\mathrm{d}\mu_{1,\mathbf{P}^*}}{\mathrm{d}\mu_{0}} \in \mathcal{H},$$
 (h^*)

we then have

$$\max_{h} R_{\mathcal{P}}(h) = D_{\mathrm{KL}}(\mu_0, \mu_{1, \mathbf{P}^*}),$$

where the maximum is obtained at h^* .

Our choice of the prior set ${\mathcal P}$

$$H_0: Y_t \overset{i.i.d.}{\sim} \mu_0 \ \forall t \in [n]$$
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▶ Why called regular? $\mu_0 \in \mathcal{P}_{\Delta}|_{\Delta=0}$ so $R_{\mathcal{P}}(h) = 0$ for any h.

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$$\sup_{\boldsymbol{P}\in\mathcal{P}_{\Delta}}\phi_{h}(\boldsymbol{P}):=\mathbb{E}_{1}[\mathrm{e}^{-h(Y)}|\boldsymbol{P}] \ \ \text{where} \ \ \mathcal{P}_{\Delta}=\{\boldsymbol{P}=(P_{1},\cdots,P_{K}):\max_{k}P_{k}\leq1-\Delta\}.$$

To verify the (\mathbf{P}^{\star}) condition, we show that

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To verify the (\mathbf{P}^*) condition, we show that

- ▶ For any non-decreasing h, $P \mapsto \phi_h(P)$ is convex in P.
- Let $\pi(\mathbf{P})$ denote the distribution whose kth coordinate is $P_{\pi(k)}$.

Extreme points of
$$\mathcal{P}_{\Delta} = \left\{ \pi(\boldsymbol{P}_{\Delta}^{\star}) : \pi \text{ is a permutation on } \{1, 2, \dots, |\mathcal{W}|\} \right\},$$

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▶ The score function $h_{gum,\Delta}^*$ is increasing:

$$h_{\mathrm{gum},\Delta}^{\star}(y) = \log \frac{\mathrm{d}\mu_{1,\mathbf{P}_{\Delta}^{\star}}}{\mathrm{d}\mu_{0}}(y) = \log \left(\left\lfloor \frac{1}{1-\Delta} \right\rfloor y^{\frac{\Delta}{1-\Delta}} + y^{\frac{\widetilde{\Delta}}{1-\widetilde{\Delta}}} \right).$$

where

$$\widetilde{\Delta} = 1 - (1 - \Delta) \cdot \left\lfloor \frac{1}{1 - \Delta} \right
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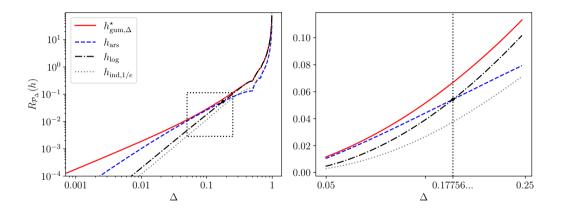
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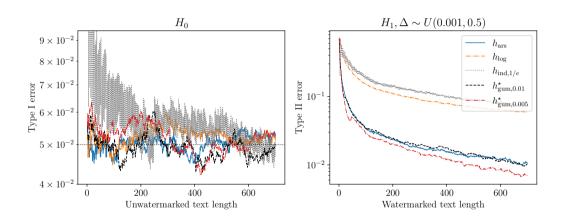
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 \implies The optimal score function is $h_{\text{gum},\Delta}^{\star}$.



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Outline

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Analysis of μ_0 and $\mu_{1,P}$ for inverse transform watermark

Lemma

ightharpoonup Recall $\eta(i) := \frac{i-1}{|\mathcal{W}|-1}$. Under H_0 , the CDF of Y_t^{dif} is

$$\mathbb{P}_0(Y_t^{\mathrm{dif}} \leq r) = rac{1}{|\mathcal{W}|} \sum_{i=1}^{|\mathcal{W}|} \left[\min\{\eta(i) + r, 1\} - \max\{\eta(i) - r, 0\}
ight]. \quad (\mu_0)$$

• Under H_1 , the conditional CDF of Y_t^{dif} is

$$\mathbb{P}_1(Y_t^{\mathrm{dif}} \leq r | \boldsymbol{P}_t) = \frac{1}{|\mathcal{W}|!} \sum_{\boldsymbol{\pi}} \sum_{i=1}^{|\mathcal{W}|} |(\boldsymbol{a}_{\boldsymbol{\pi},i-1}, \boldsymbol{a}_{\boldsymbol{\pi},i}] \cap B(\eta(i), r)|, \qquad (\mu_{1,\boldsymbol{P}_t})$$

where $a_{\pi,i} = \sum_{j=1}^{i} P_{t,\pi(j)}$, $B(v,r) = \{x \in [0,1] : |x-v| \le r\}$ and $|\cdot|$ represents the length of an interval.

Analysis of μ_0 and $\mu_{1,P}$ for inverse transform watermark

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➤ A complicated combinatorial structure due to the permutation.

Weak convergence of CDFs

Key observation

Only dominant probabilities in ${m P}$ matters. Simplify formulation by asymptotic analysis.

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Only dominant probabilities in \boldsymbol{P} matters. Simplify formulation by asymptotic analysis.

Theorem

Under H_0 ,

$$\lim_{|\mathcal{W}| o \infty} \mathbb{P}_0(Y_t^{\mathrm{dif}} \leq y) = 1 - (1-y)^2 \;\; ext{for any} \;\; y \in [0,1].$$

 $\textit{Under H}_1, \textit{ assuming that } \lim_{|\mathcal{W}| \to \infty} P_{t,(1)} = 1 - \Delta \textit{ and } \lim_{|\mathcal{W}| \to \infty} \log |\mathcal{W}| \cdot P_{t,(2)} = 0 \textit{ hold,}$

$$\lim_{|\mathcal{W}| o \infty} \mathbb{P}_1(Y_t^{ ext{dif}} \leq y \mid extbf{ extit{P}}_t) = 1 - \left(1 - rac{y}{1 - \Delta}
ight)^2 \quad ext{for any } \ y \in [0, 1 - \Delta]. \qquad (\mu_{1, \Delta})$$

Limit efficiency measure

▶ Let $K = |\mathcal{W}|$. For any log $K \cdot \varepsilon_K \to 0$, we define

$$\overline{P}_{\Delta} = \left\{ \mathbf{P} : P_{(1)} \leq 1 - \Delta, \ P_{(2)} \leq \varepsilon_K \right\}.$$

▶ The asymptotic perspective leads to the following limit efficiency measure:

$$\overline{R}_{\Delta}(h) = \liminf_{K \to \infty} R_{\overline{P}_{\Delta}}(h).$$

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▶ Under some technical conditions, we can exchange the order of liminf, sup, inf, so

$$\overline{R}_{\Delta}(h) = -\inf_{ heta \geq 0} \left\{ heta \mathbb{E}_{\mu_0} h(Y^{ ext{dif}}) + \sup_{\Delta_0 \geq \Delta} \log \mathbb{E}_{\mu_{1,\Delta_0}} [e^{- heta h(Y^{ ext{dif}})}]
ight\}.$$

Finding optimal detection rule is reduced to solve the minimax optimization problem:

$$\sup_h \overline{R}_{\Delta}(h) = -\inf_h \left\{ \mathbb{E}_{\mu_0} h(Y^{\mathrm{dif}}) + \sup_{\Delta_0 > \Delta} \log \phi_h(\Delta_0) \right\} \ \, \text{where} \, \, \phi_h(\Delta_0) := \mathbb{E}_{\mu_{1,\Delta_0}}[e^{-h(Y^{\mathrm{dif}})}].$$

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- ▶ For (P^*) , $\sup_{\Delta_0 \ge \Delta} \phi_h(\Delta_0) := \phi_h(\Delta)$ for all any non-increasing and Lipschitz h.
- ▶ For (h^*) , the score function $h^*_{\text{dif},\Delta}$ is decreasing and local Lipschitz:

$$h_{\mathrm{dif},\Delta}^{\star}(y) = \log rac{f_{\mathrm{dif},\Delta}(y)}{f_{\mathrm{dif},0}(y)} \;\; ext{where} \;\; f_{\mathrm{dif},\Delta}(y) = rac{2}{1-\Delta} \cdot \max \left\{ 1 - rac{y}{1-\Delta}, 0
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 \implies The optimal score function is $h_{\text{dif}, \Lambda}^{\star}$.

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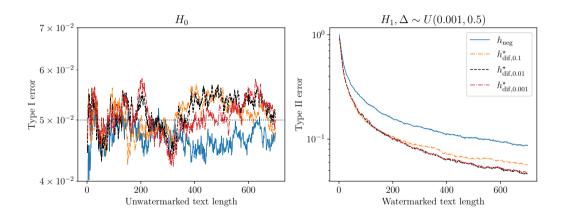
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- \implies The optimal score function is $h_{\text{dif},\Delta}^{\star}$.
 - !! $\sup_h \overline{R}_{\Delta}(h) = \infty$. Be cautious to interpret this result.

Simulation results



Efficiency comparison on C4 newslike dataset and OPT-1.3B

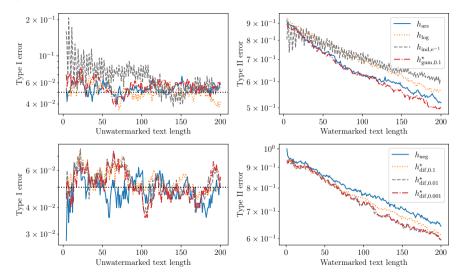


Figure: Left: Type I. Right: Type II. Top: Gumbel-max. Bottom: Inverse transform.

Outline

Introduction

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Summary

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- A statistical framework for detecting unbiased watermarks.
- Define the least-favorable efficiency measure to compare different detection rules.
- Identify the optimal detection rule according to the efficiency measure.

Future work

- Robust detection methods.
- Compare different watermarks or pivots.
- Analysis for biased watermarks.
- ► Failure of working hypothesis.

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