

# Theoretically Grounded Framework for LLM Watermarking: A Distribution-Adaptive Approach

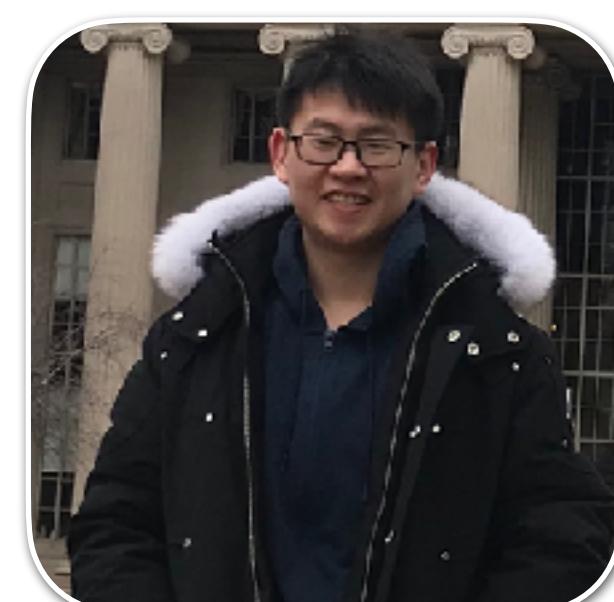
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ITA 2025



Yepeng Liu  
Univ. of Florida



Prof. Ziqiao Wang  
Tongji Univ.



Prof. Yongyi Mao  
Univ. of Ottawa



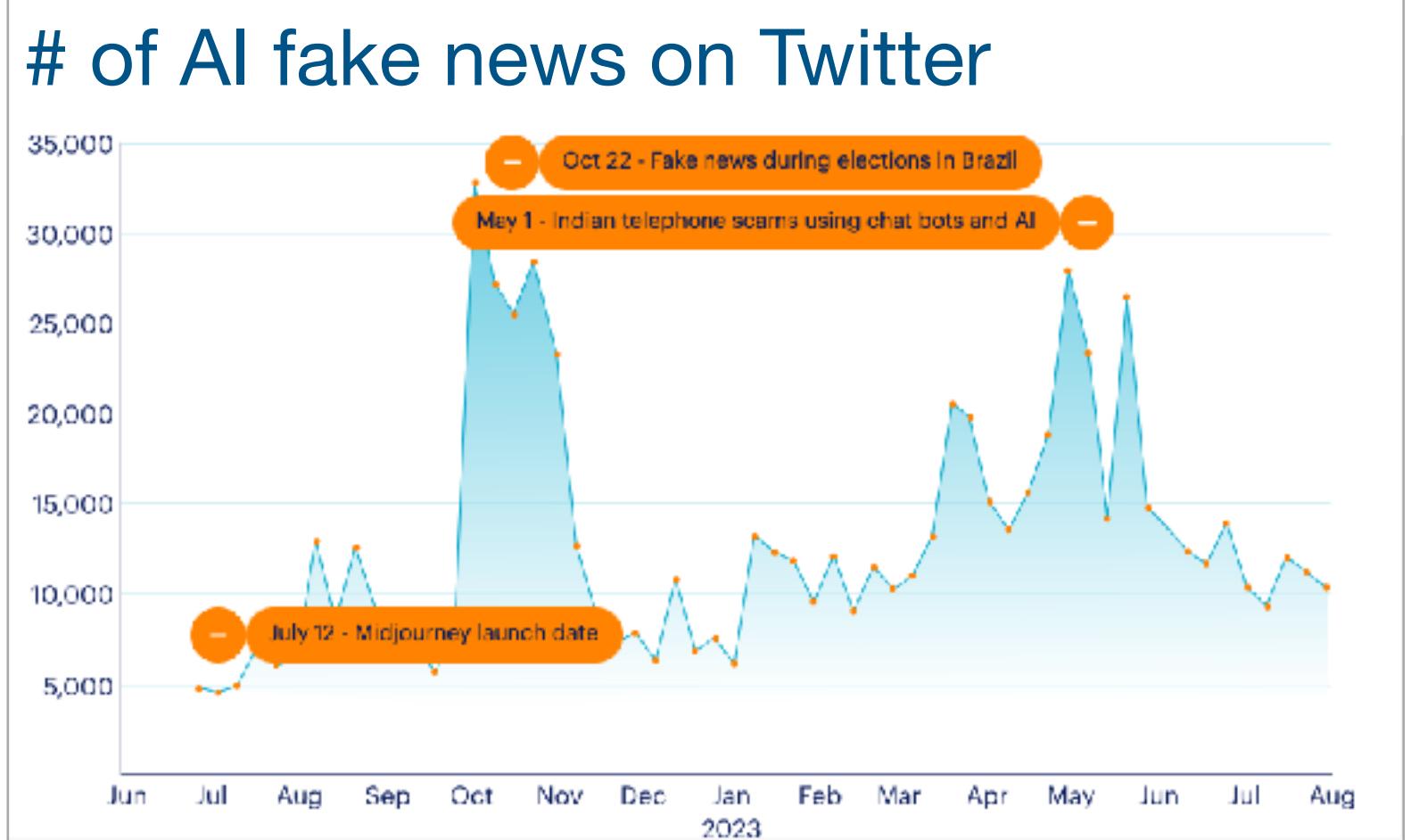
Prof. Yuheng Bu  
Univ. of Florida

# Challenges in AI Safety

**Misuse of AI-generated content**

# Challenges in AI Safety

## Misuse of AI-generated content



Fake news

# Challenges in AI Safety

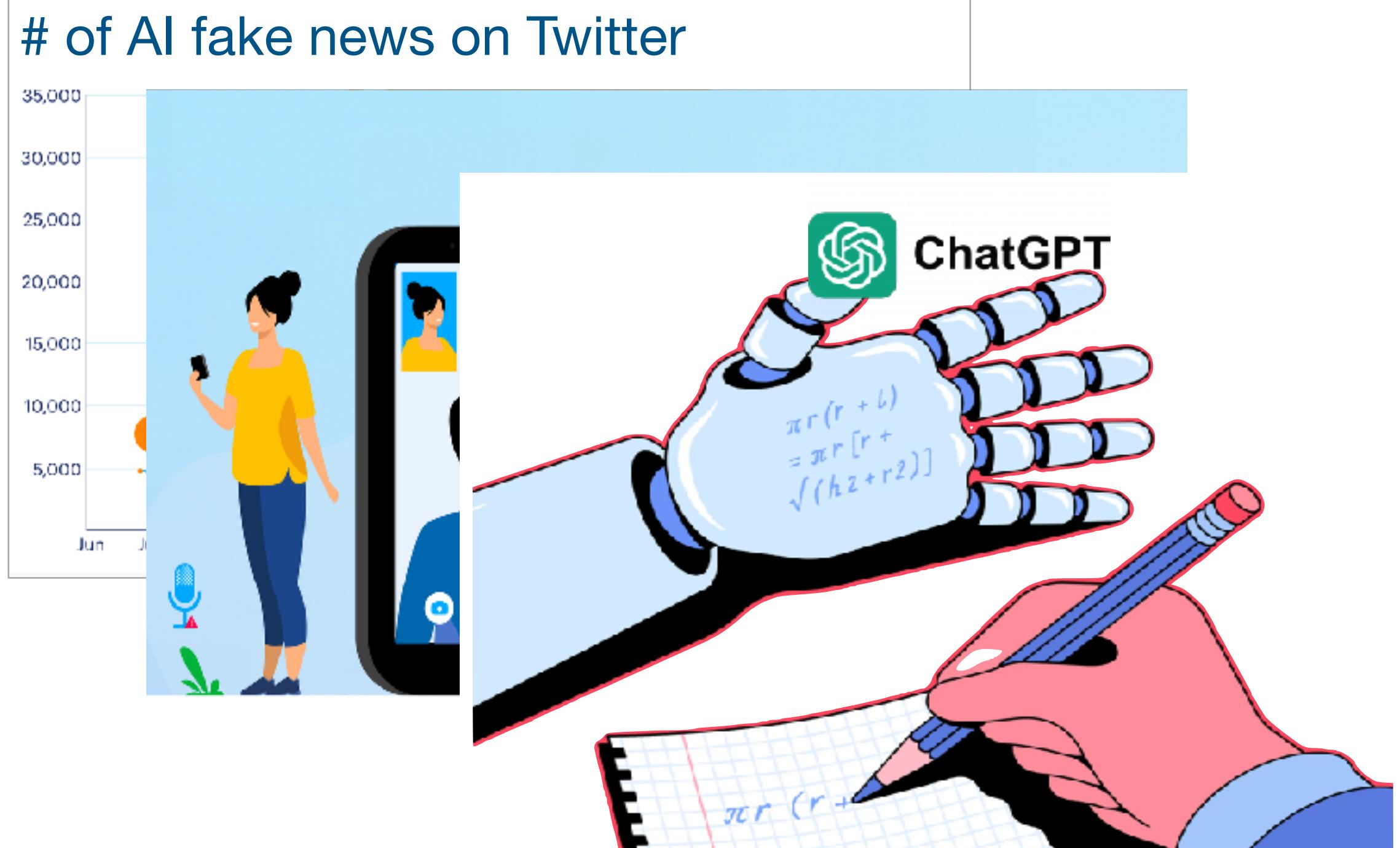
## Misuse of AI-generated content



AI scams

# Challenges in AI Safety

## Misuse of AI-generated content



# Challenges in AI Safety

## Misuse of AI-generated content

## Data Pollution



# Challenges in AI Safety

## Misuse of AI-generated content

# of AI fake news on Twitter



Plagiarism

## Data Pollution

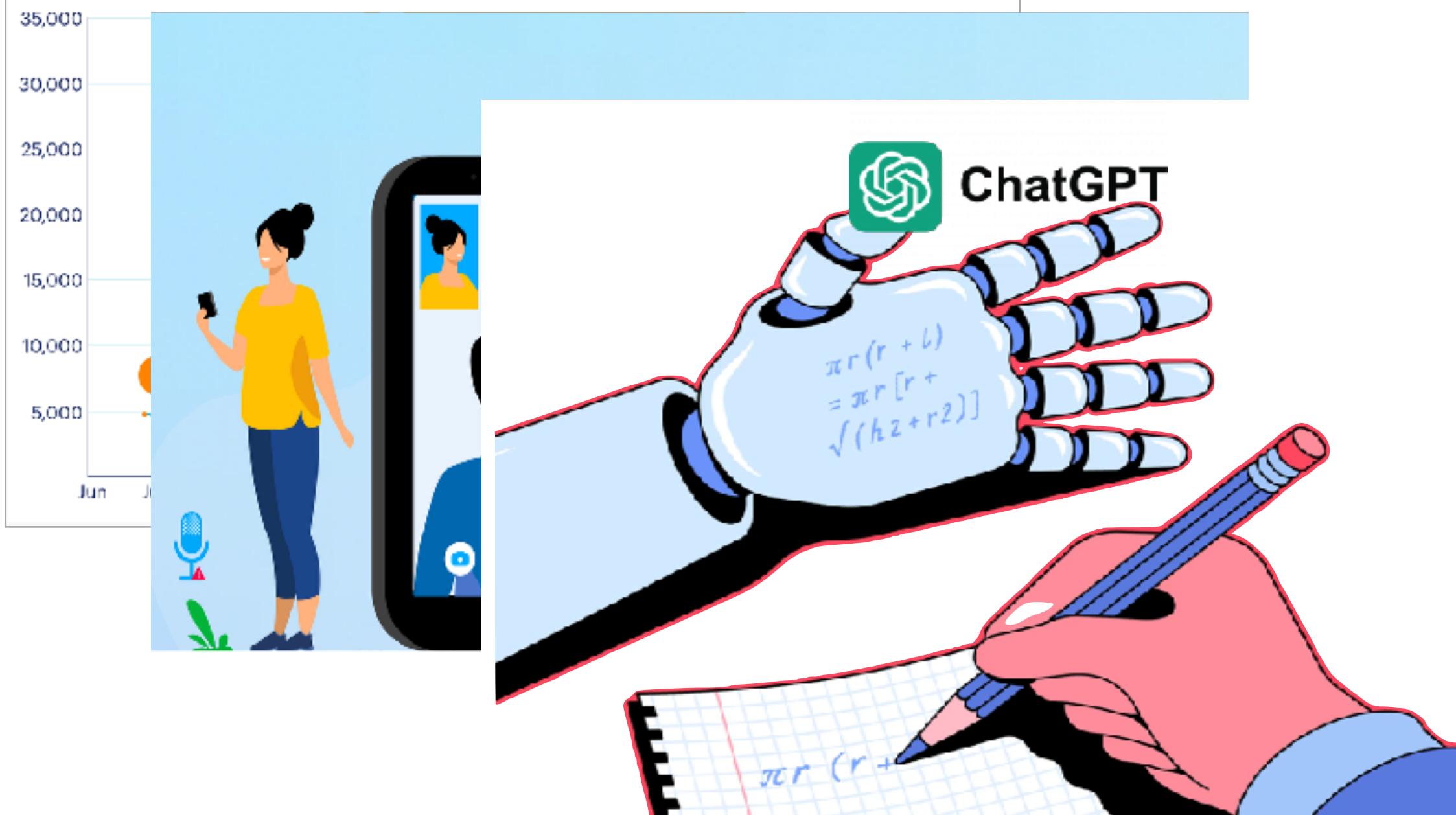
Tons of AI-generated data over the internet



# Challenges in AI Safety

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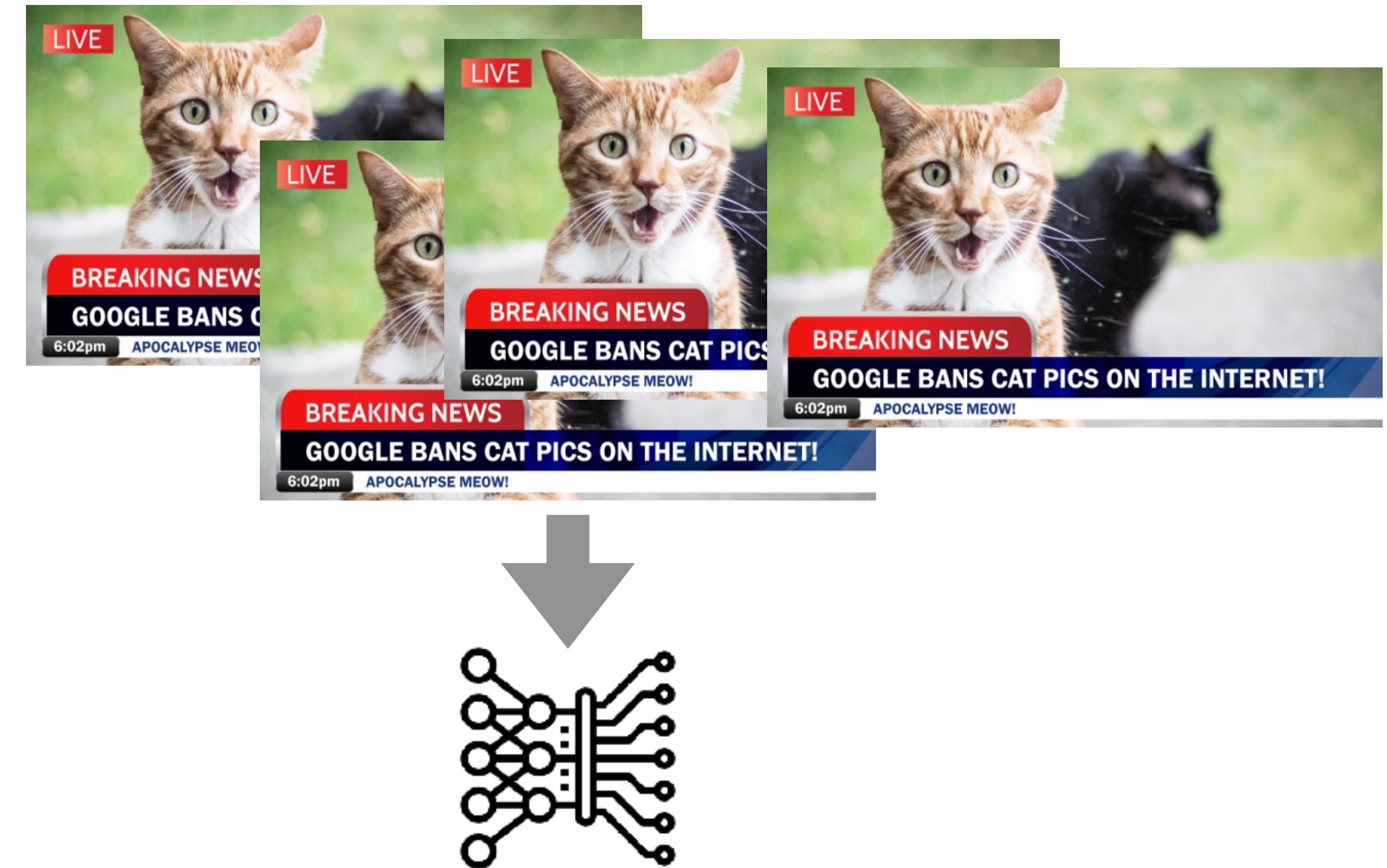
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Plagiarism

## Data Pollution

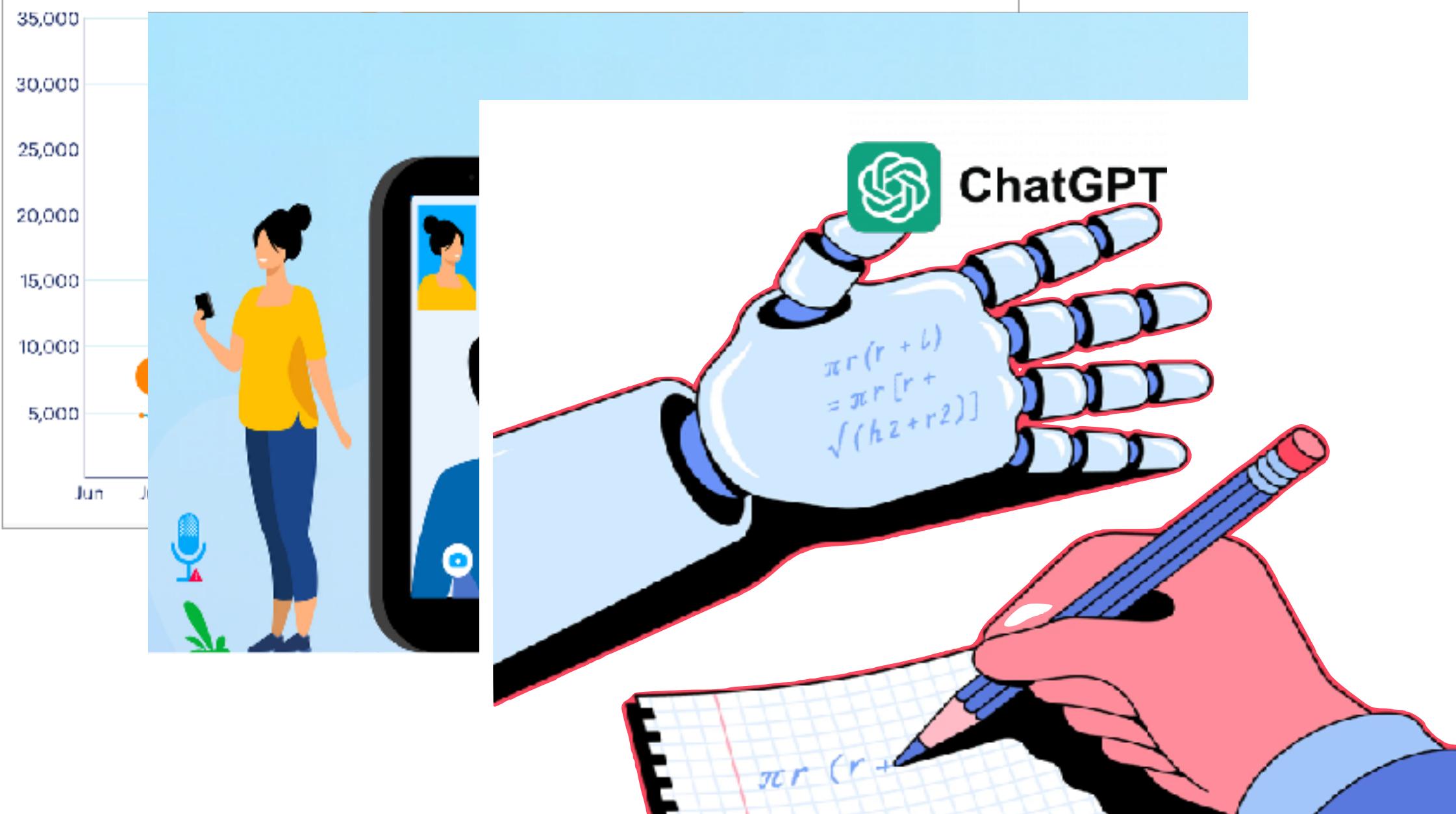
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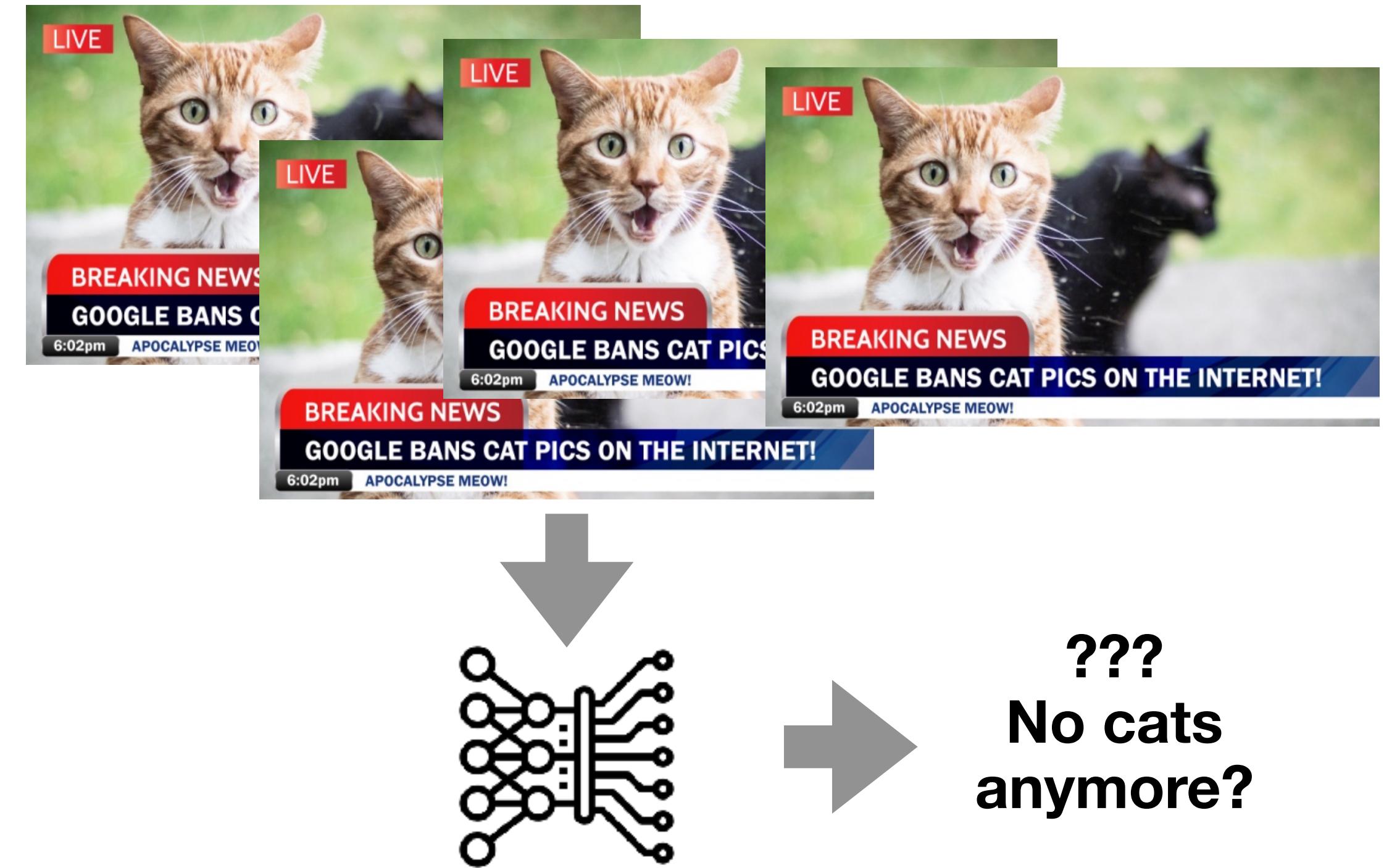
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Plagiarism

## Data Pollution

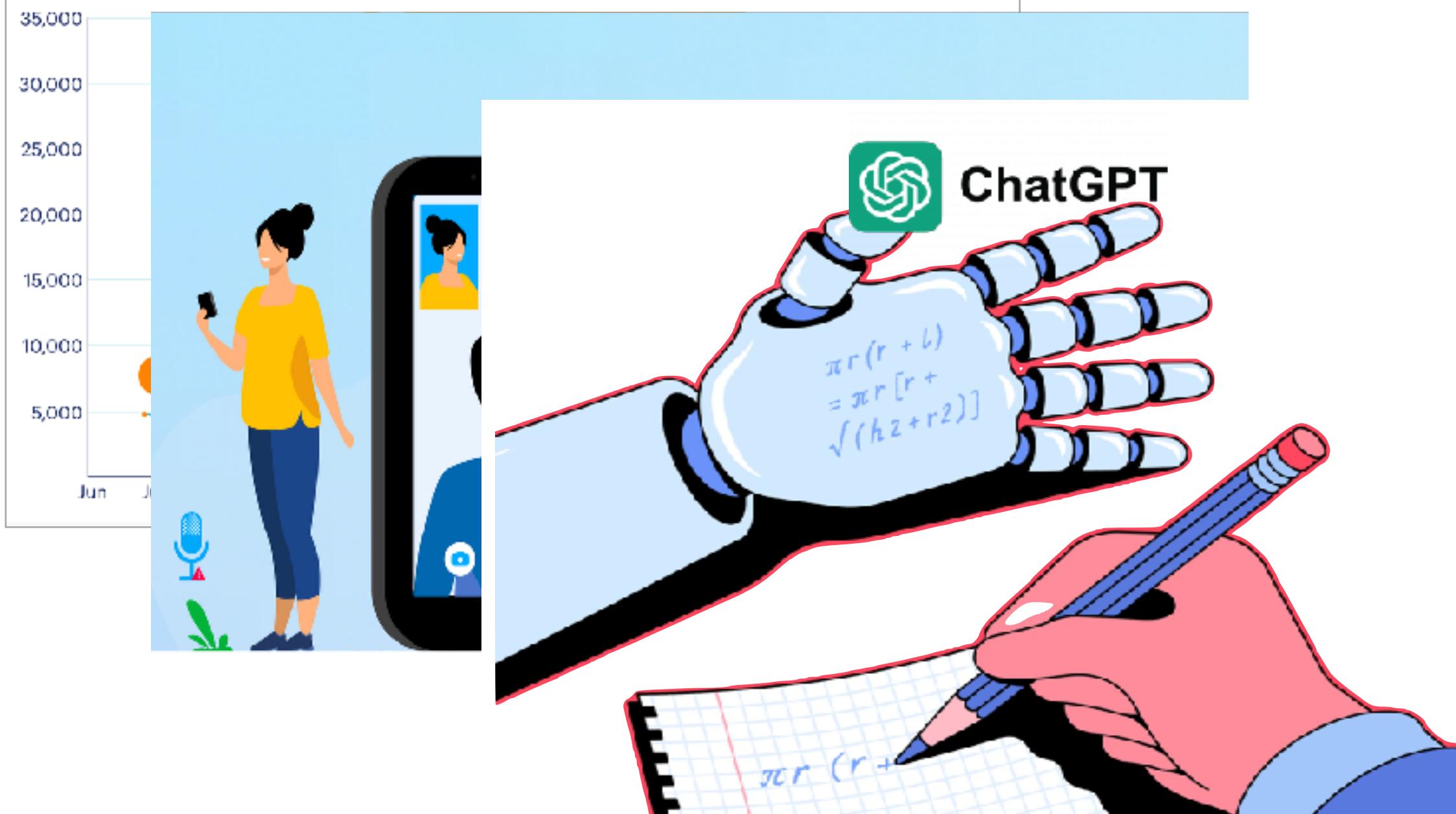
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## Misuse of AI-generated content

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Plagiarism

## Data Pollution

Tons of AI-generated data over the internet

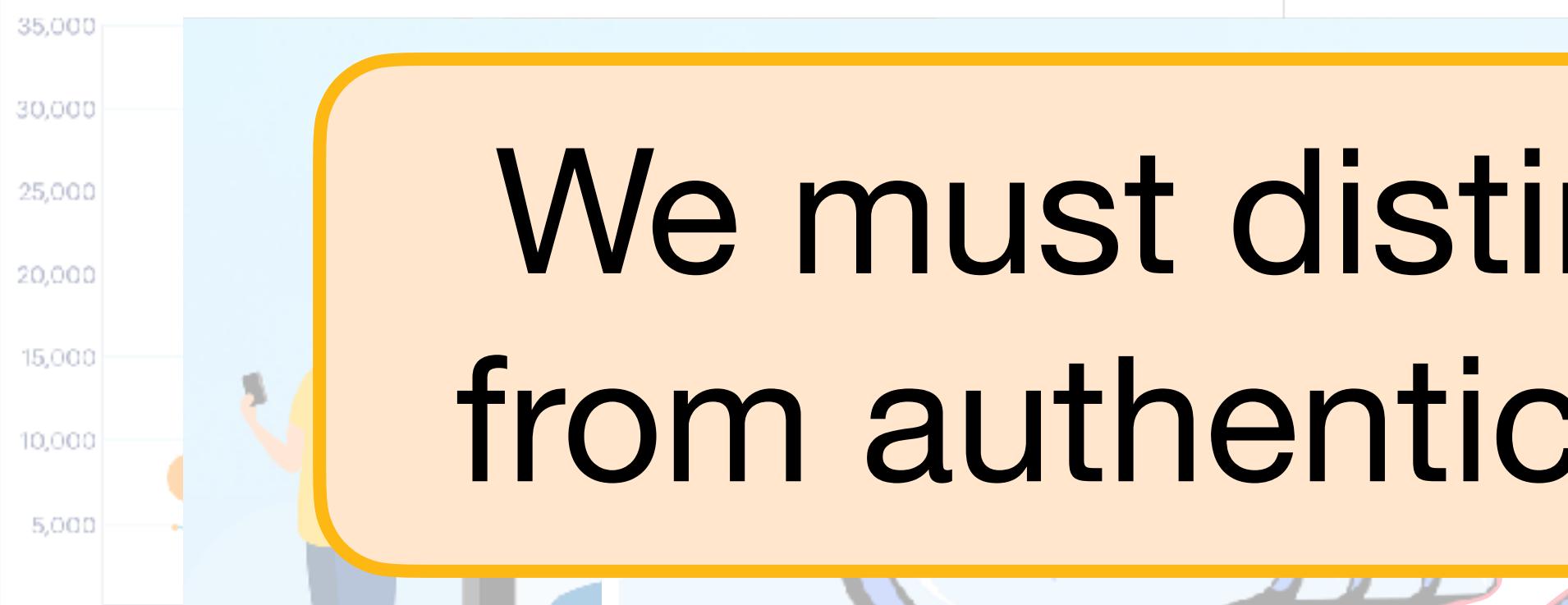


???  
No cats  
anymore?

# Challenges in AI Safety

## Misuse of AI-generated content

# of AI fake news on Twitter

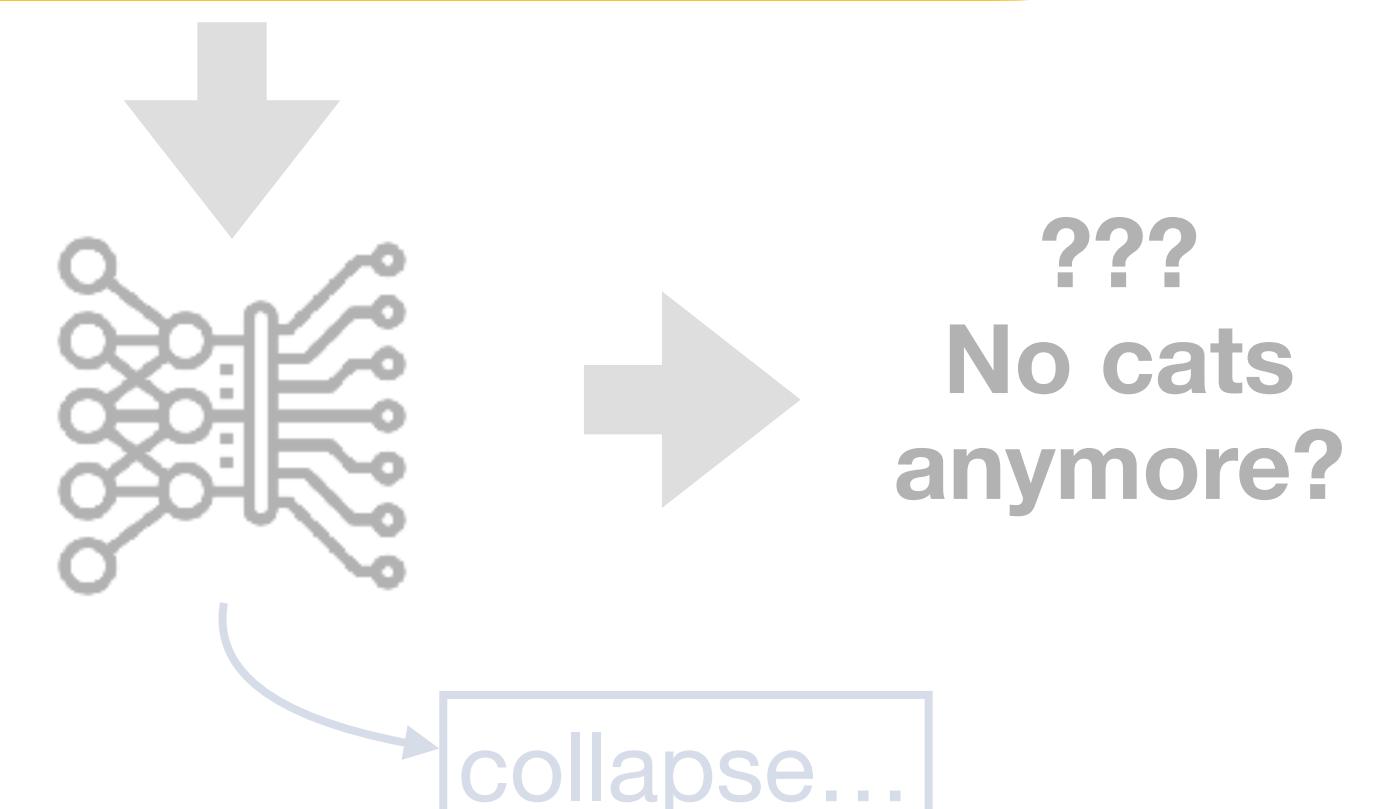
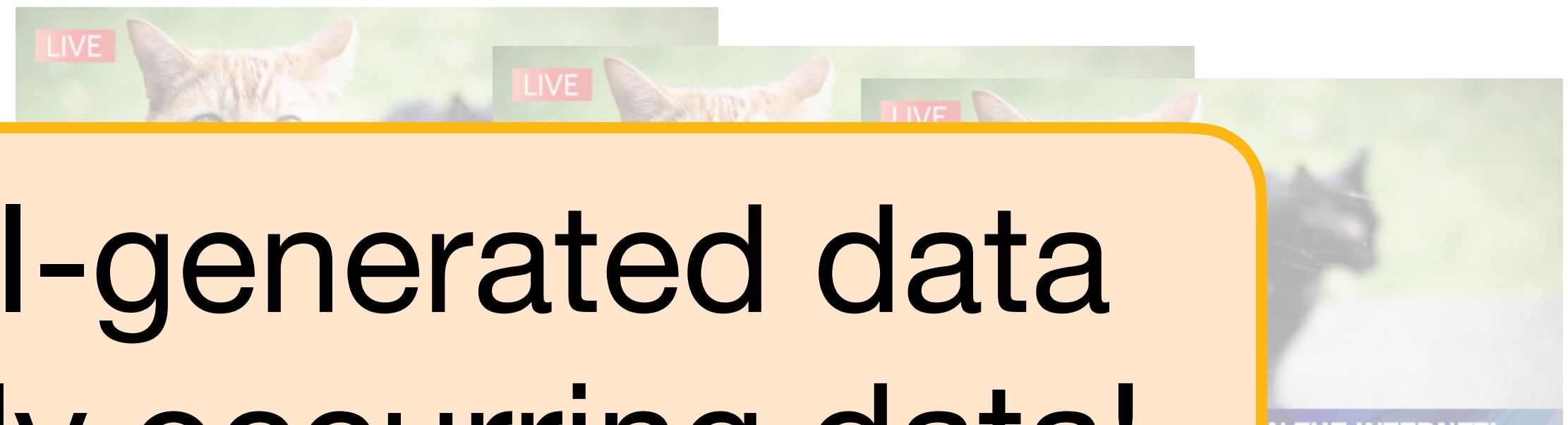


We must distinguish AI-generated data  
from authentic, naturally occurring data!

Plagiarism

## Data Pollution

Tons of AI-generated data over the internet



# Identify AI-generated Text

## Possible solutions?

# Identify AI-generated Text

## Possible solutions?

- By observation:

# Identify AI-generated Text

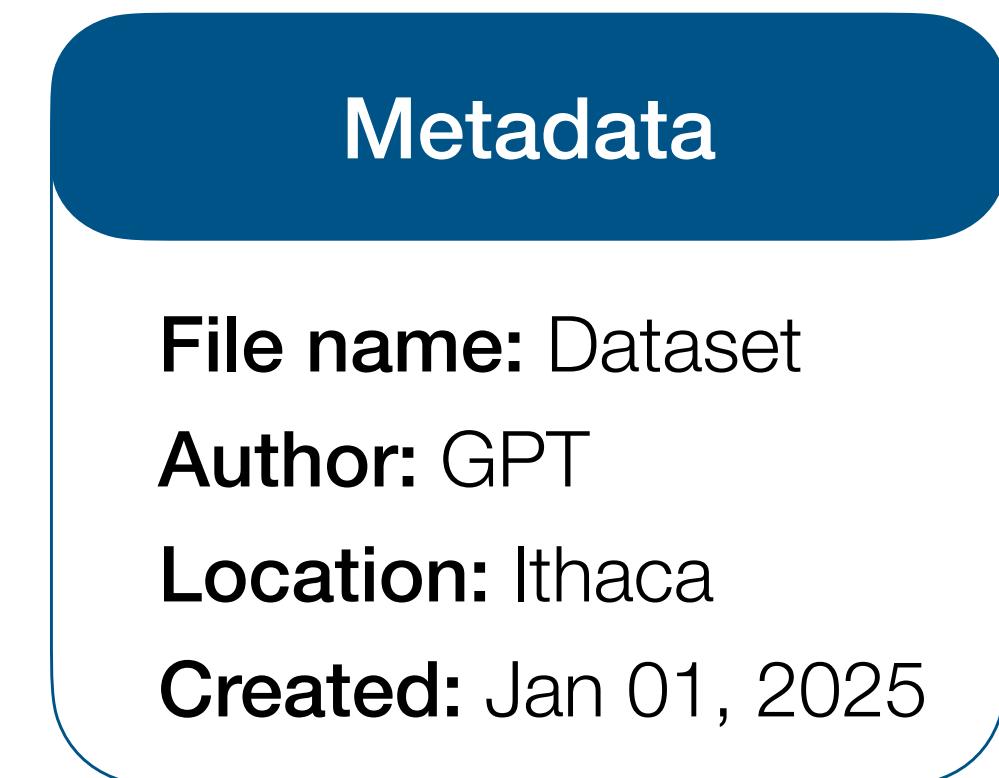
## Possible solutions?

*“Here’s the revised version of your...”, “Best regards,[Your Name]”* :-D

# Identify AI-generated Text

## Possible solutions?

- Metadata <— easy to remove



# Identify AI-generated Text

## Possible solutions?

- Giant database to store all AI-generated content <—storage? privacy?

# Identify AI-generated Text

## Possible solutions?

- Discriminator models:  **GPTZero**  DetectGPT  **Copyleaks**  **pangramlabs** ...

# Identify AI-generated Text

## Possible solutions?

<— high prob of falsely alarming human-written text

# Identify AI-generated Text

## Possible solutions?

- Watermarking: inserting a signal into LLM predicted tokens

# Identify AI-generated Text

## Possible solutions?



- **Watermarking: inserting a signal into LLM predicted tokens**

# Identify AI-generated Text

## Possible solutions?



- Watermarking: inserting a signal into LLM

Simul knows that when you are making changes to an existing document you want it saved as a new file, and probably don't want to have to remember to press 'save as' before you start editing and then 'save' every 30 minutes. So, Simul will automatically create a new version every time an edit is made to an existing document, saves as you go, word by word and gives you access to your documents anywhere, anytime.

You can access your documents offline on Simul, make changes and re-format knowing that the moment your computer or device is back online Simul will update the file for the rest of your team to see and save it in line with the version history.

If two team members happen to be working on the same document, offline, at the same time Simul has your back here too.

Each team member's file will be saved as a new version, uploaded when they are back online, and an alert is sent to the document owner that there are two new versions available to their review.

The document owner can then review the documents and merge them together at the click of a button.

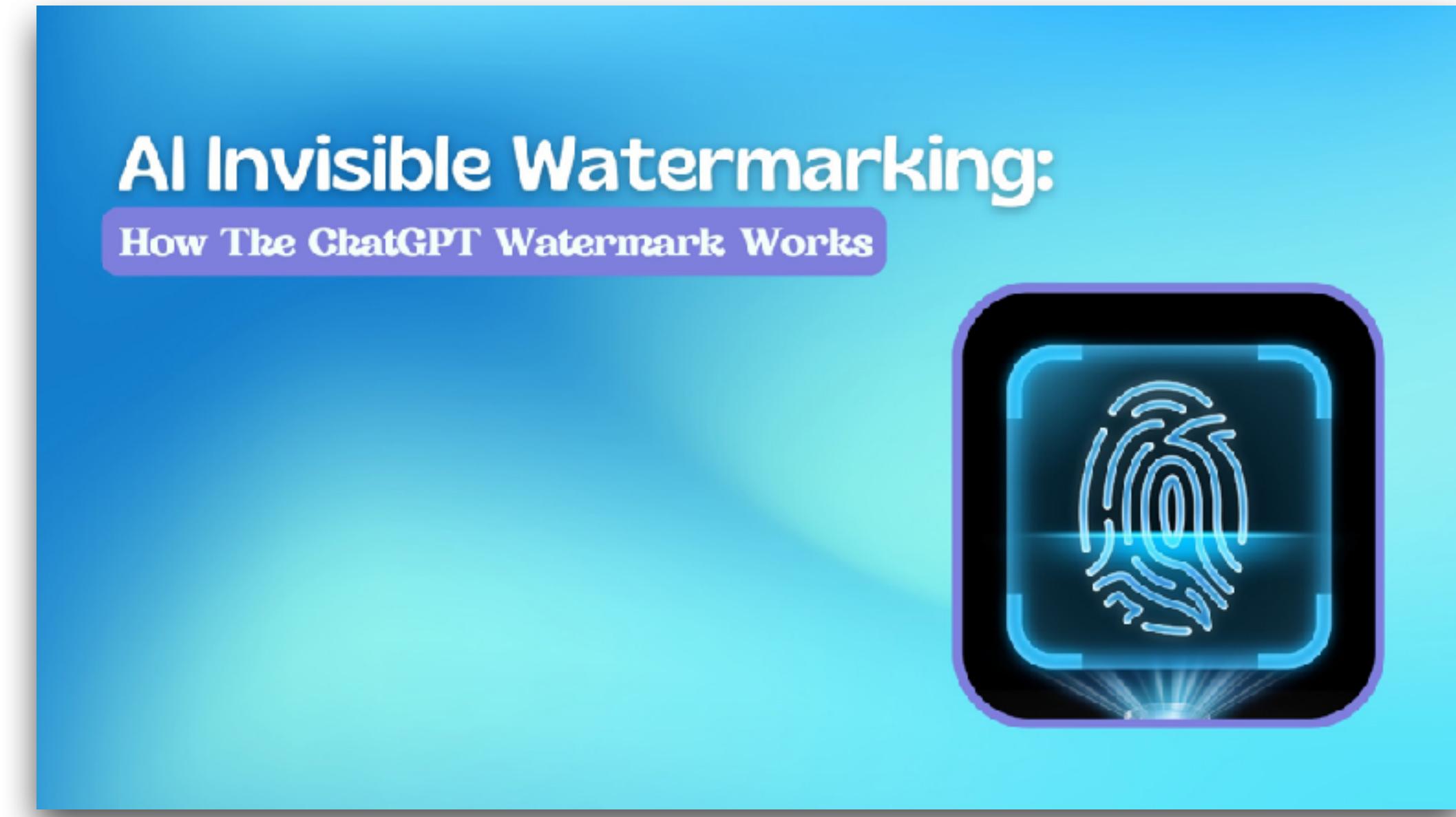
Simul allows you to collaborate from anywhere, anytime without worrying about saving your work or accidentally overriding a colleague's file.

Its collaboration made easy and Simul knows you needed it.

So, give it a try, you'll never search for a lost document again with Simul on your side.

# Identify AI-generated Text

## Possible solutions?



- **Watermarking: inserting a signal into LLM predicted tokens**

# Identify AI-generated Text

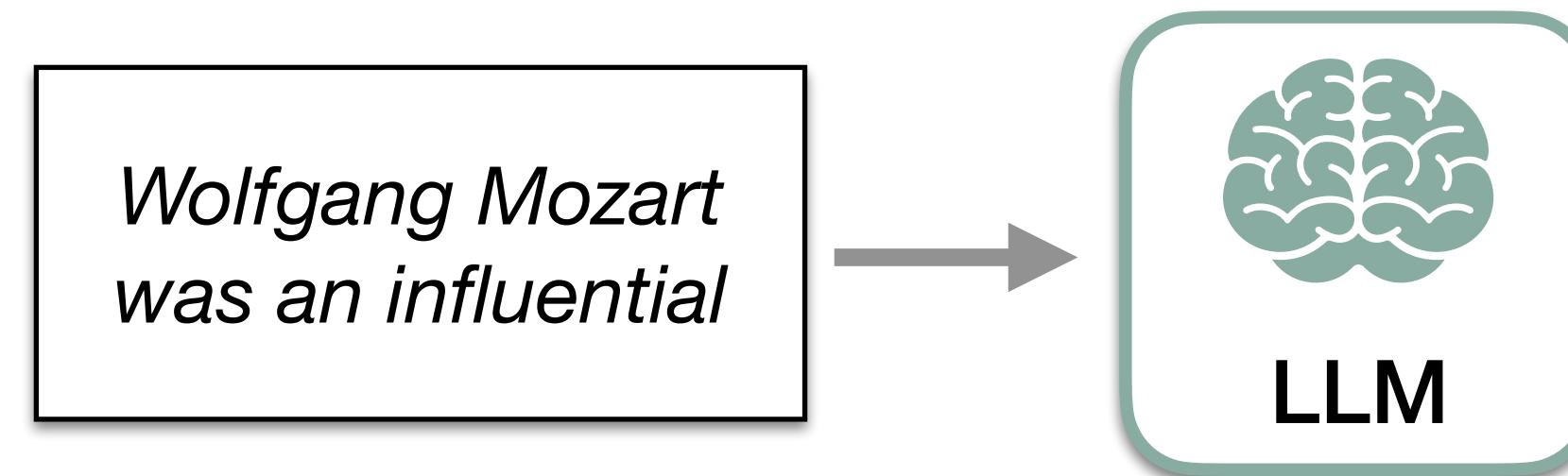
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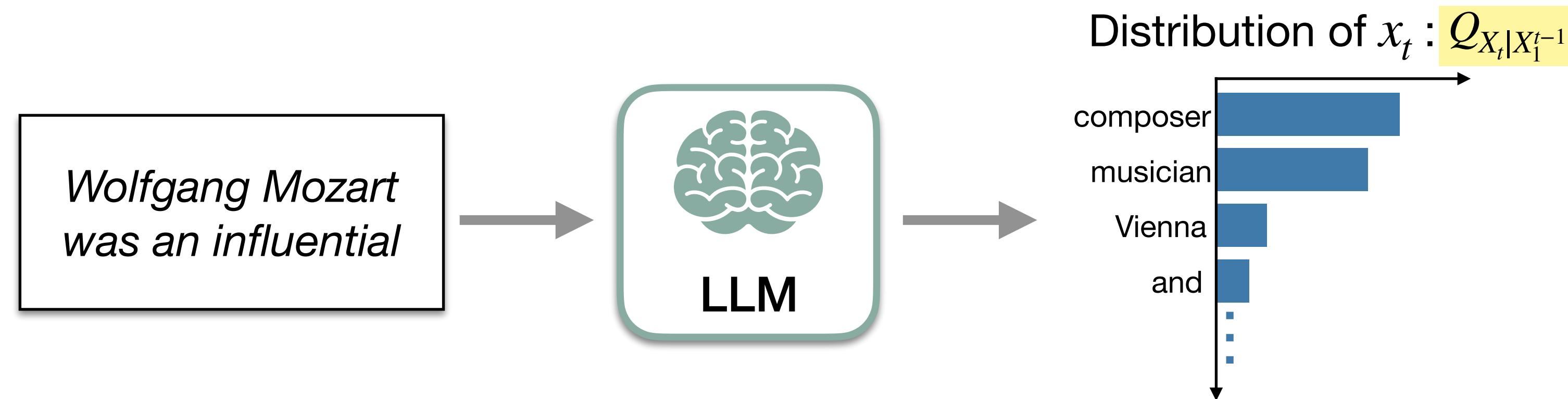


# A Framework for LLM Watermark Generation

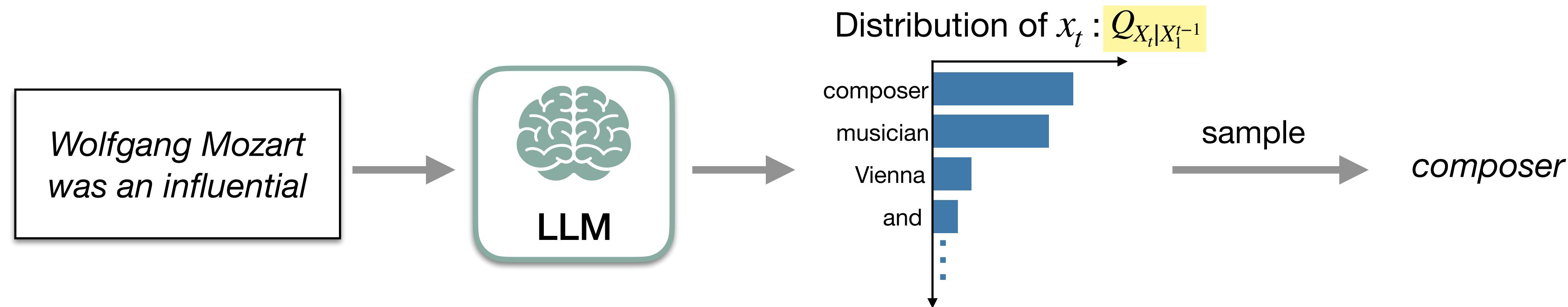
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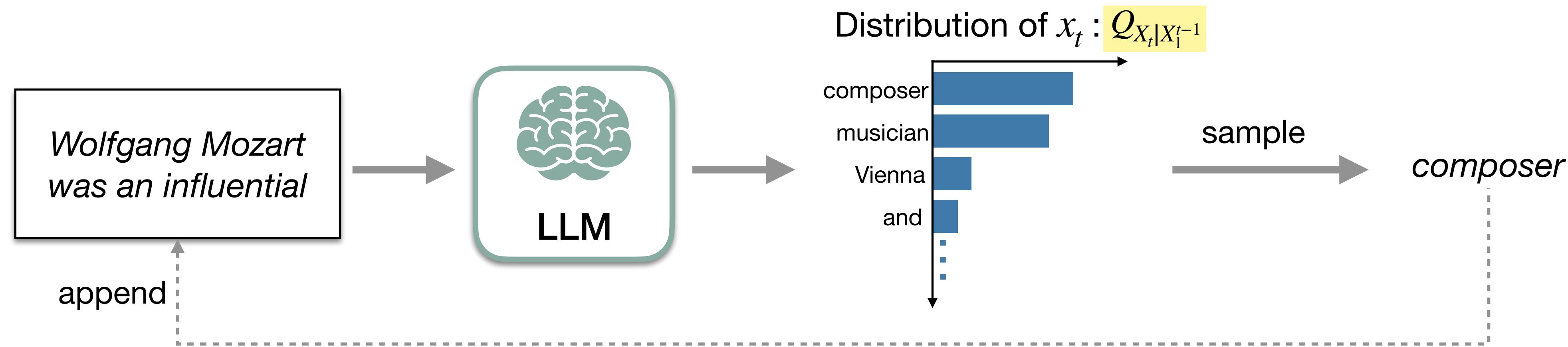
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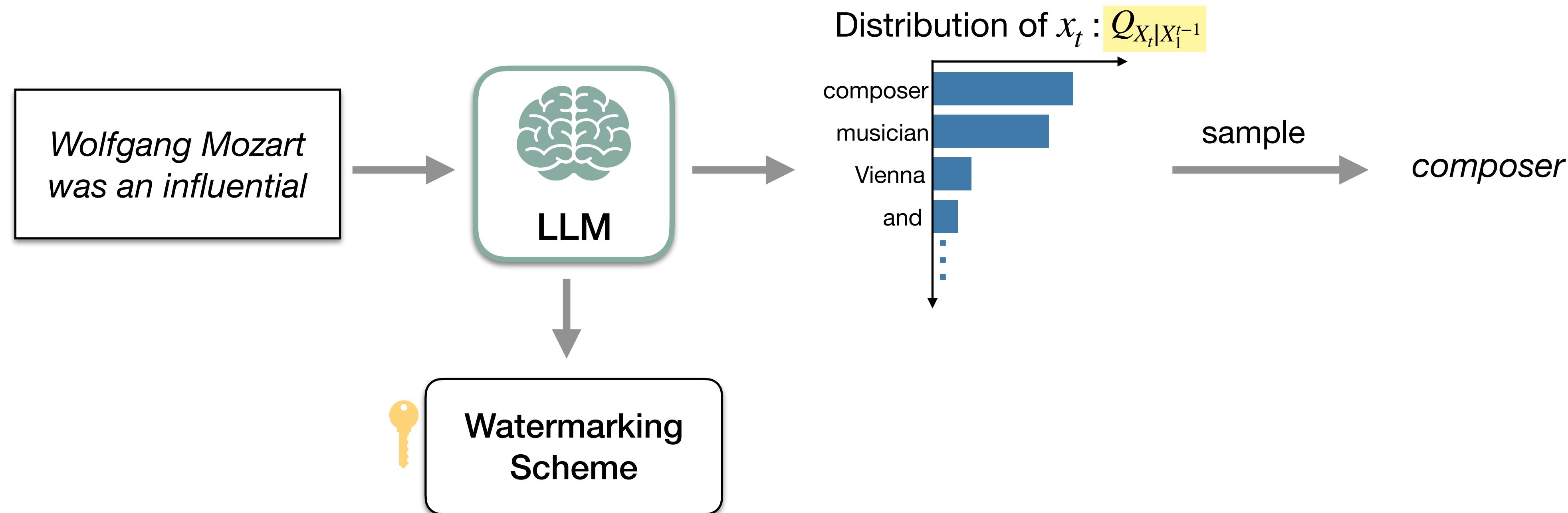
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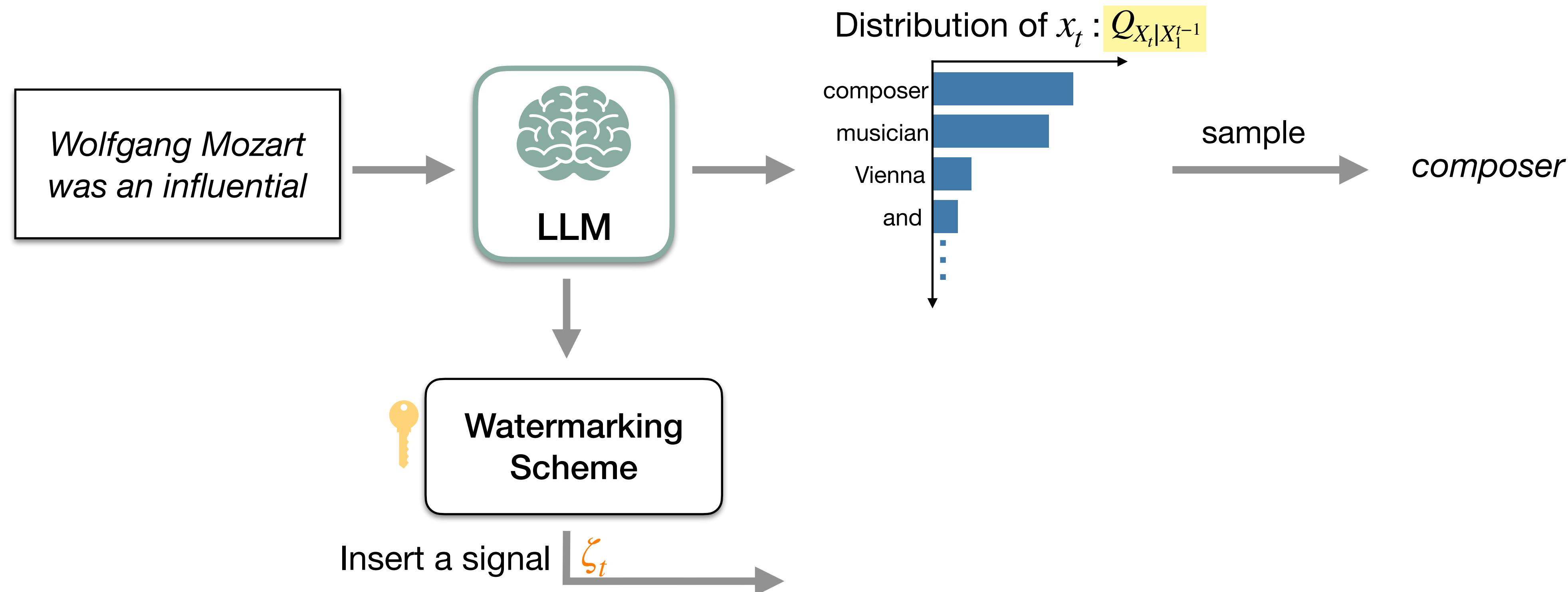
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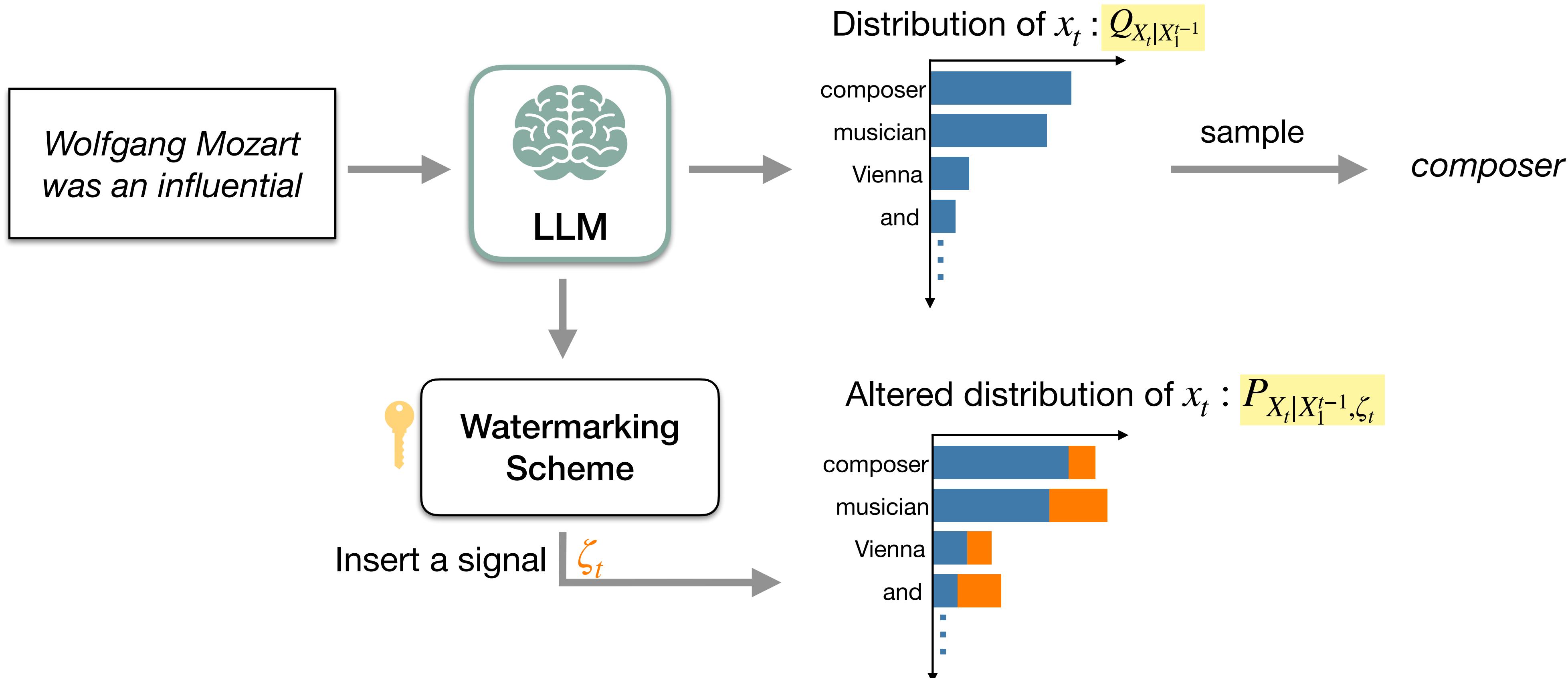
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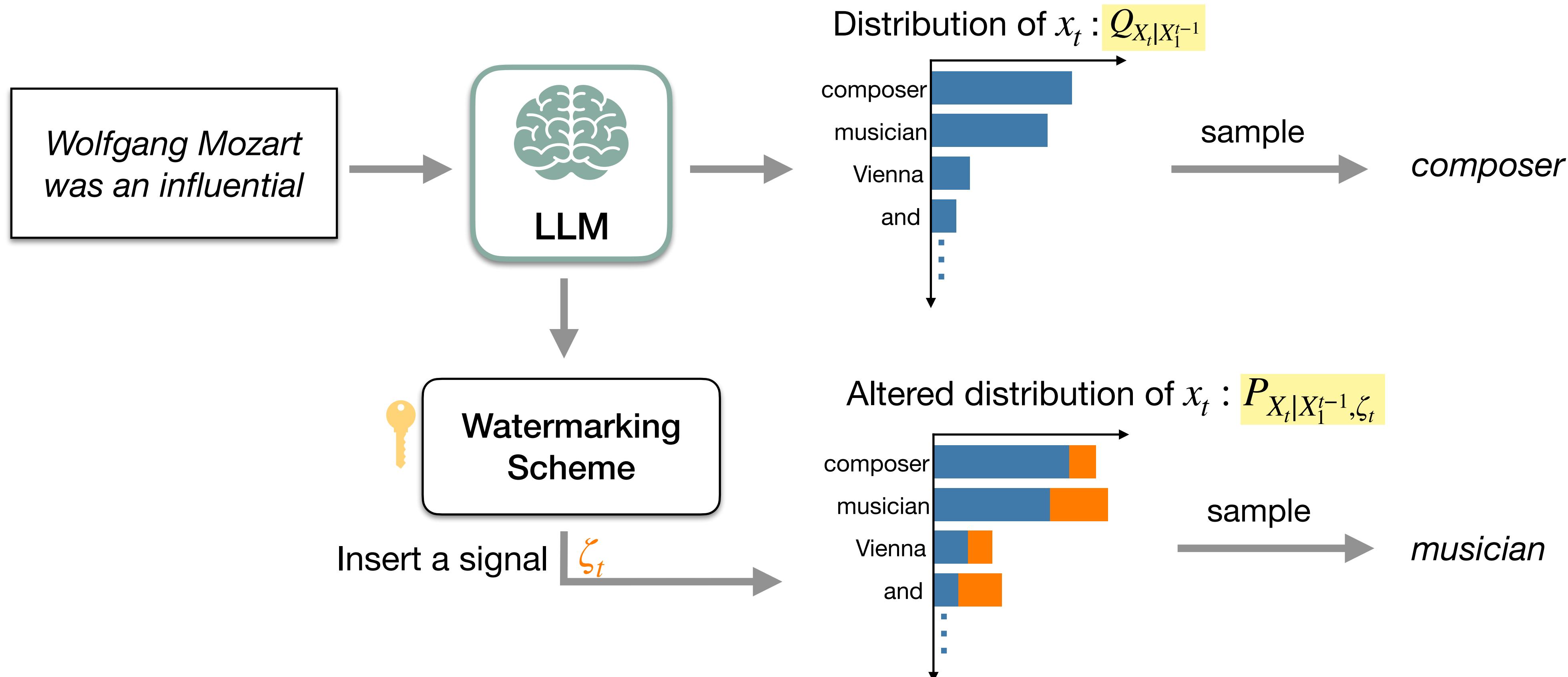
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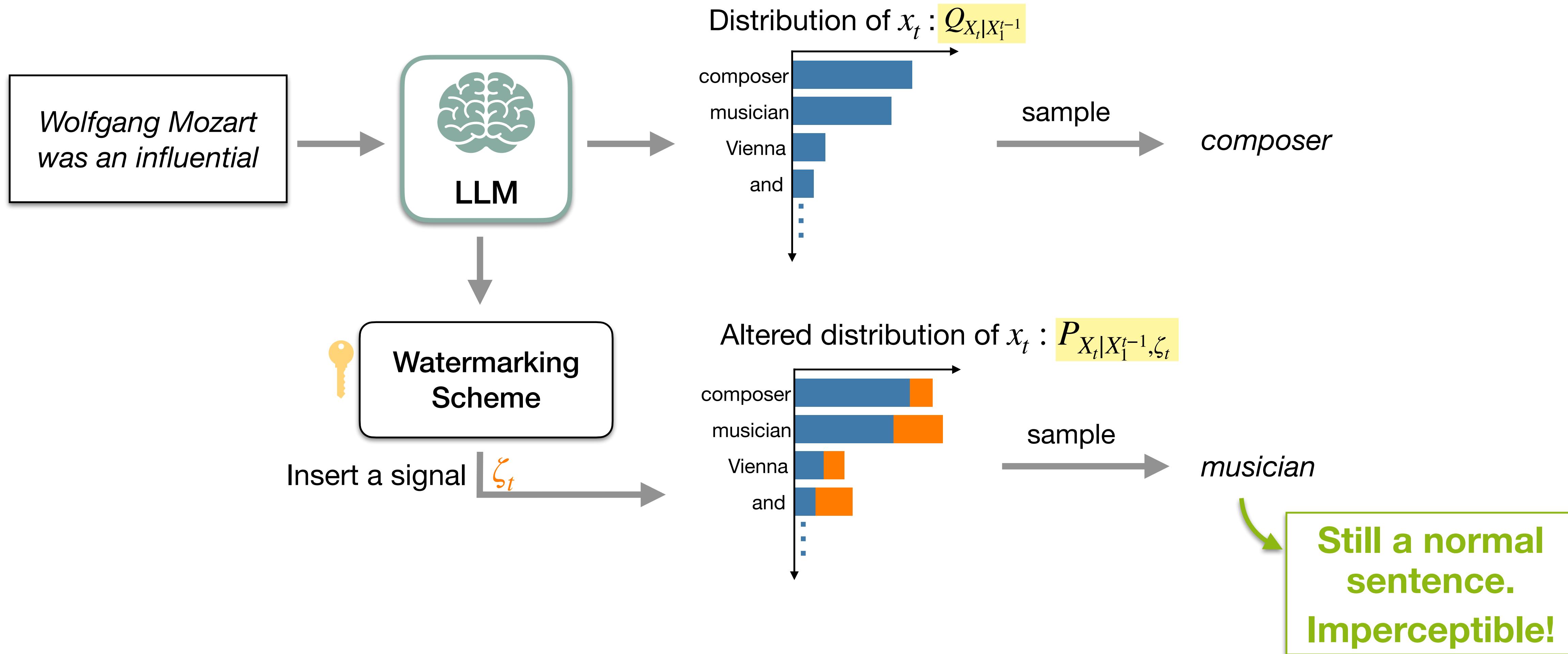
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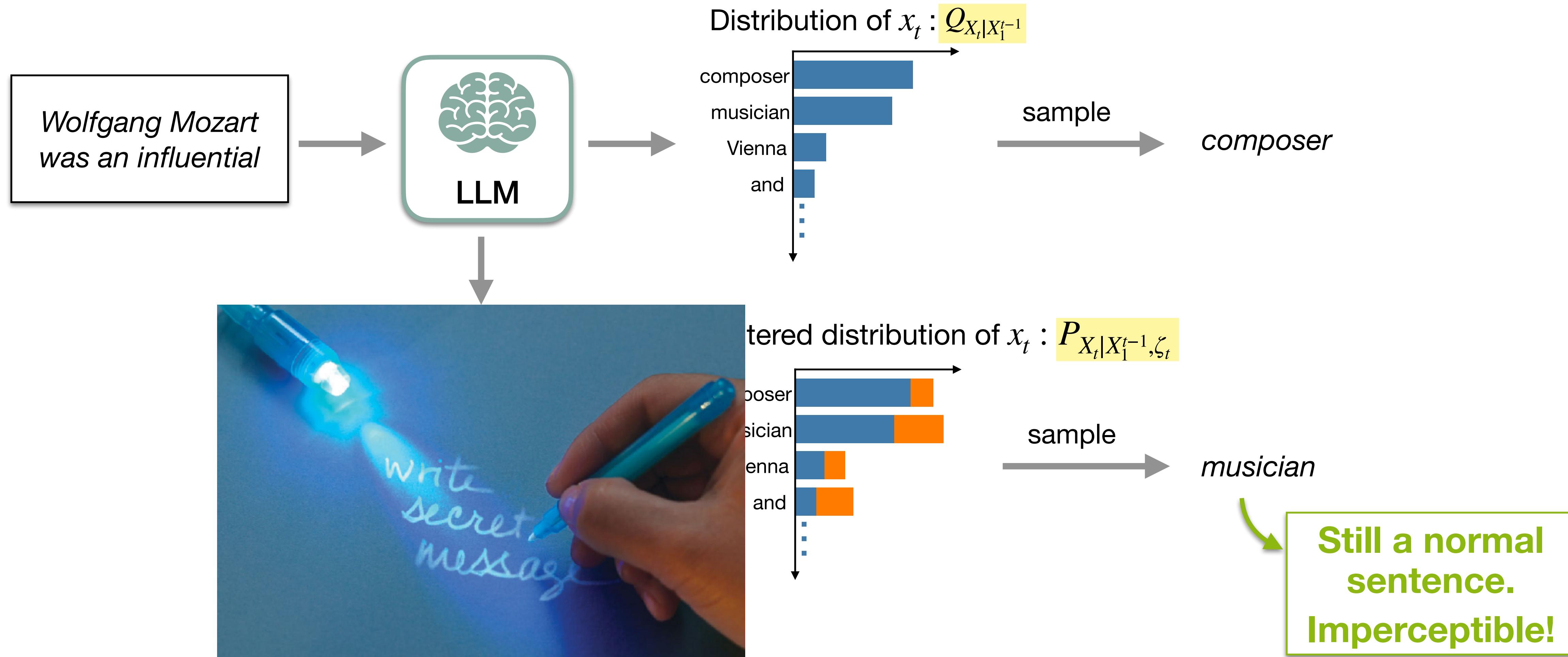
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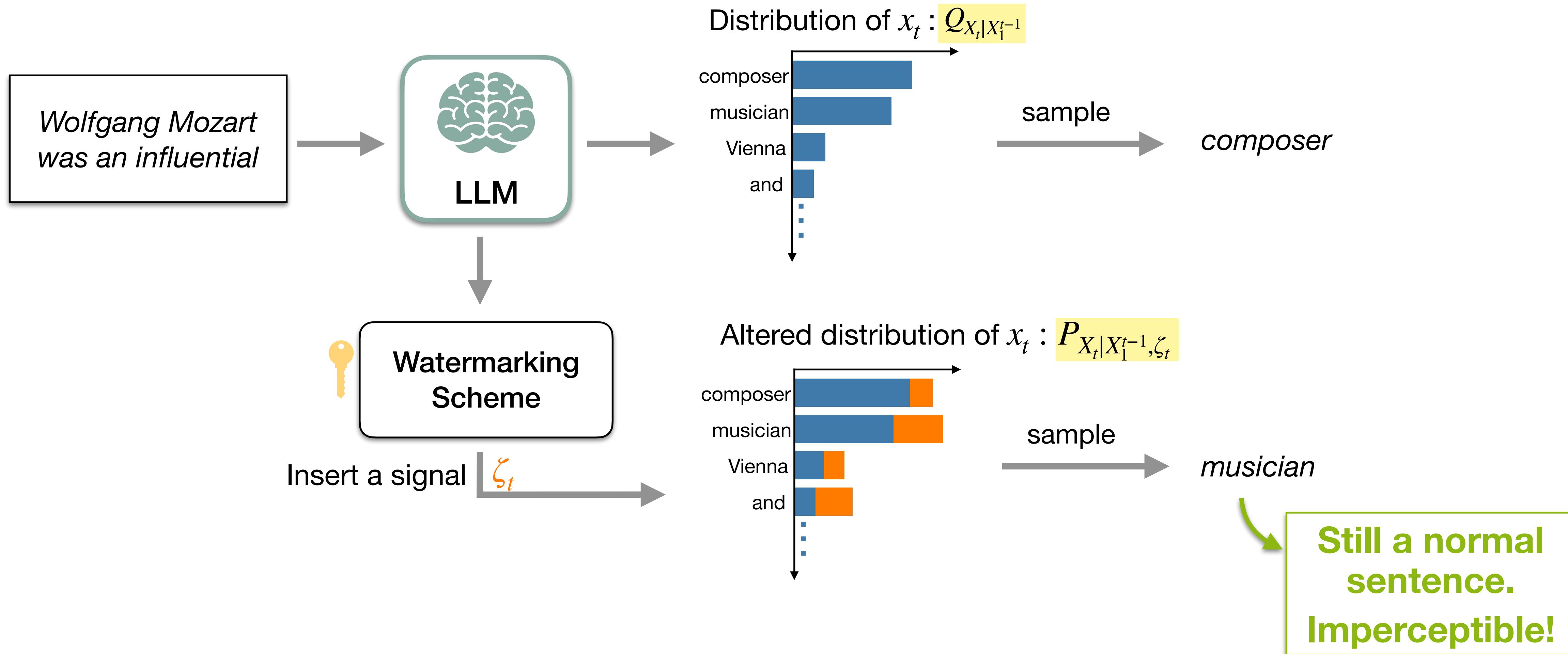


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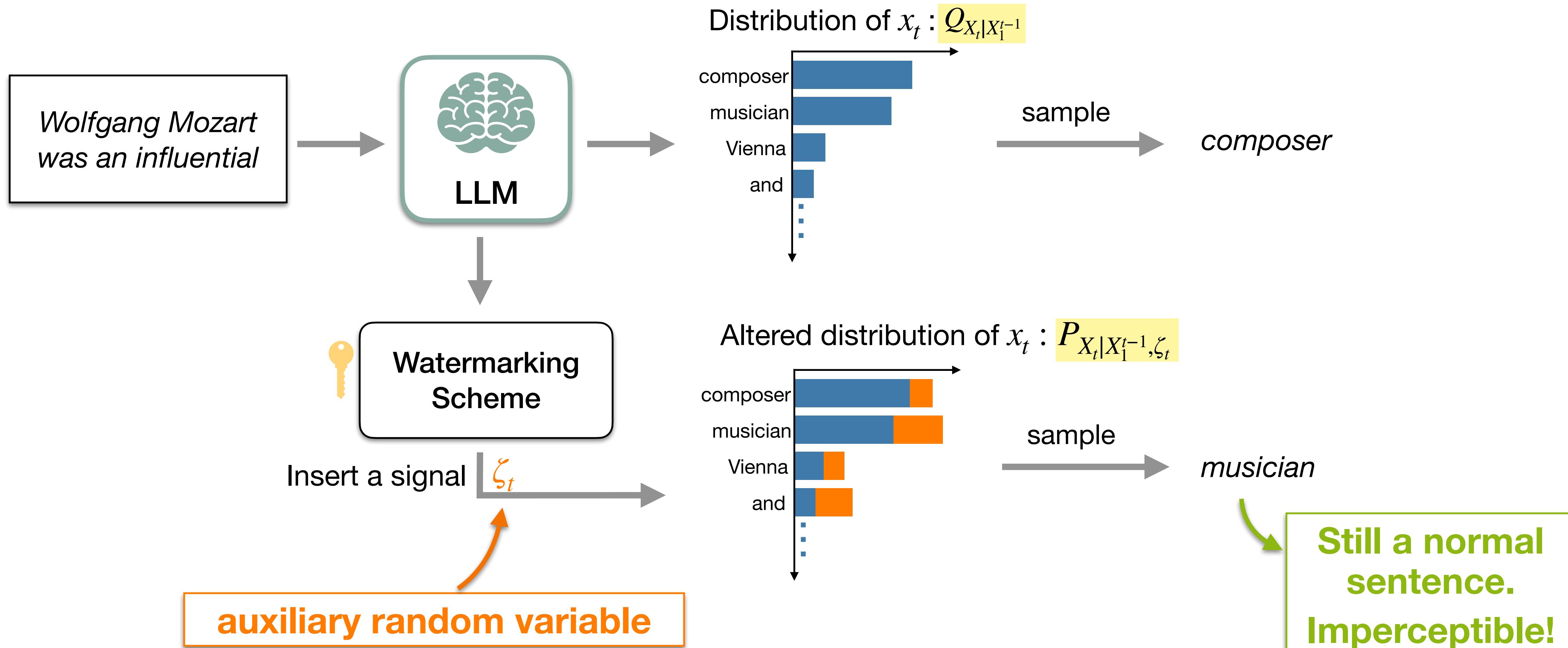


Like invisible Ink (Steganography)

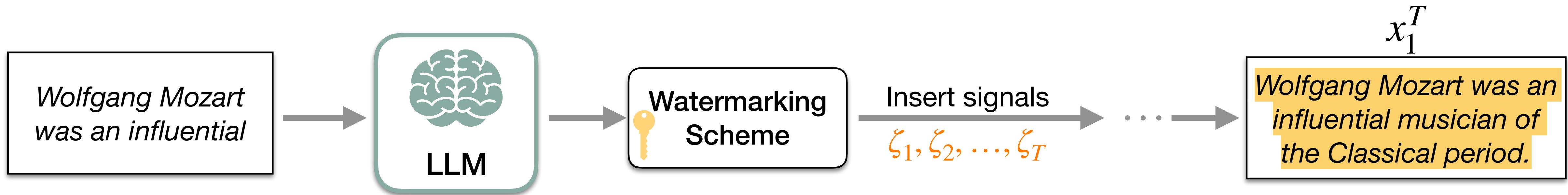
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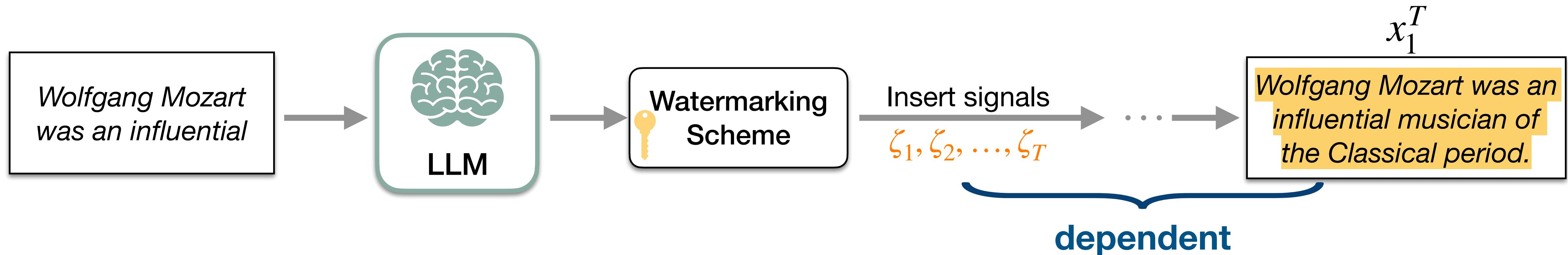
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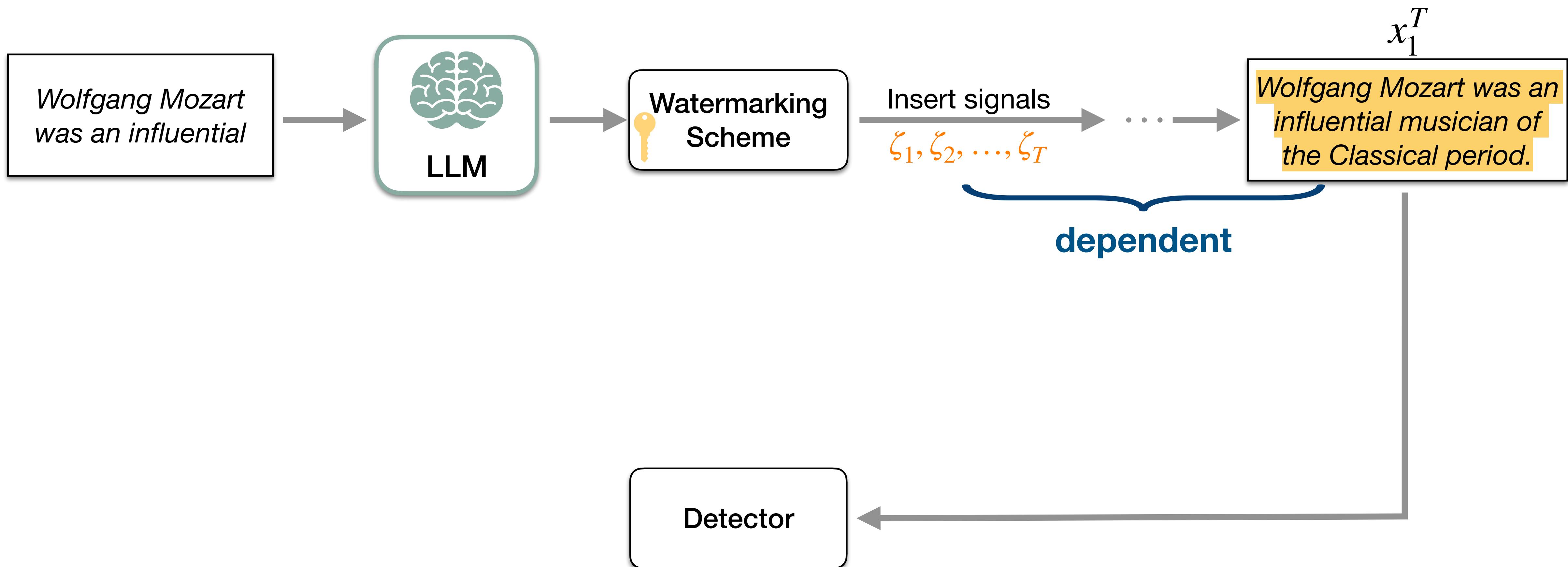
# Hypothesis Testing for LLM Watermark Detection



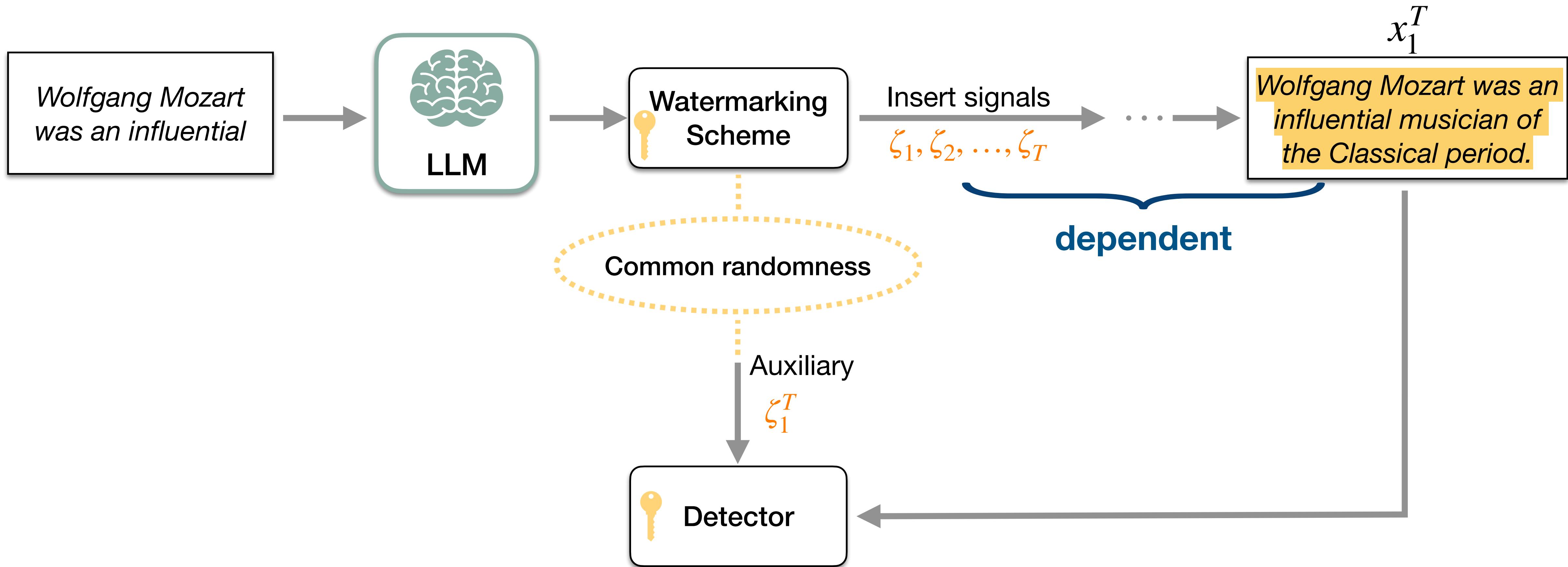
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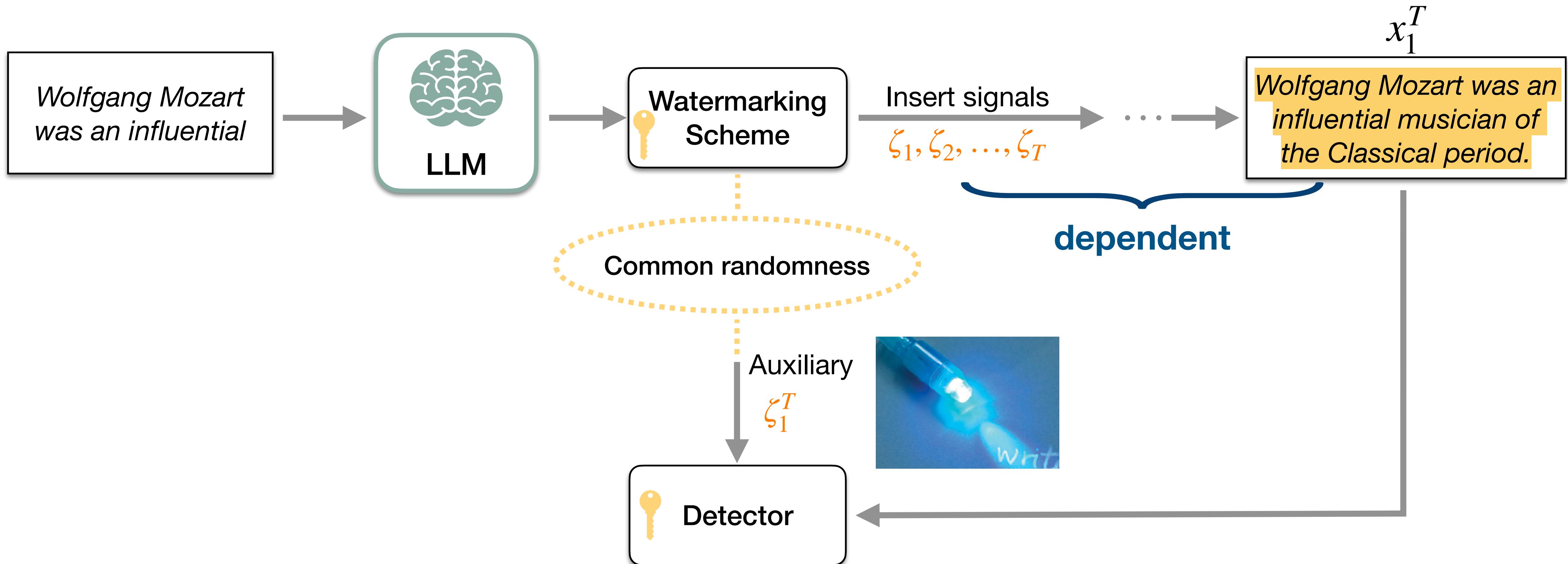
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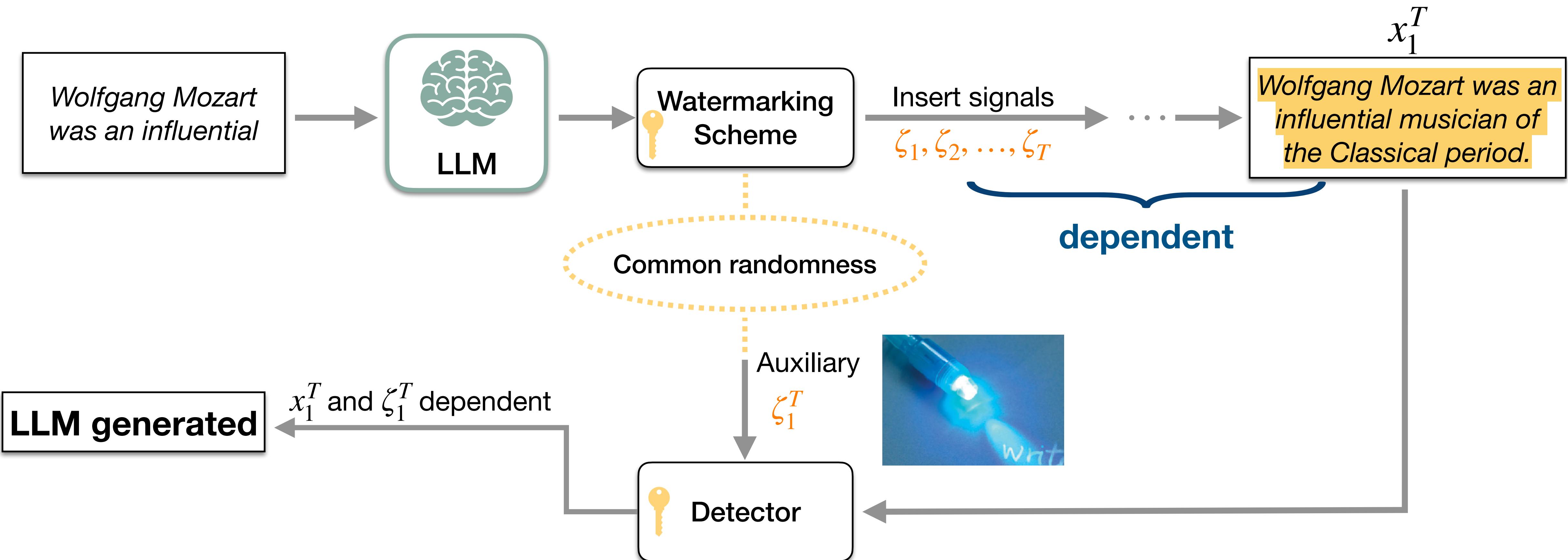
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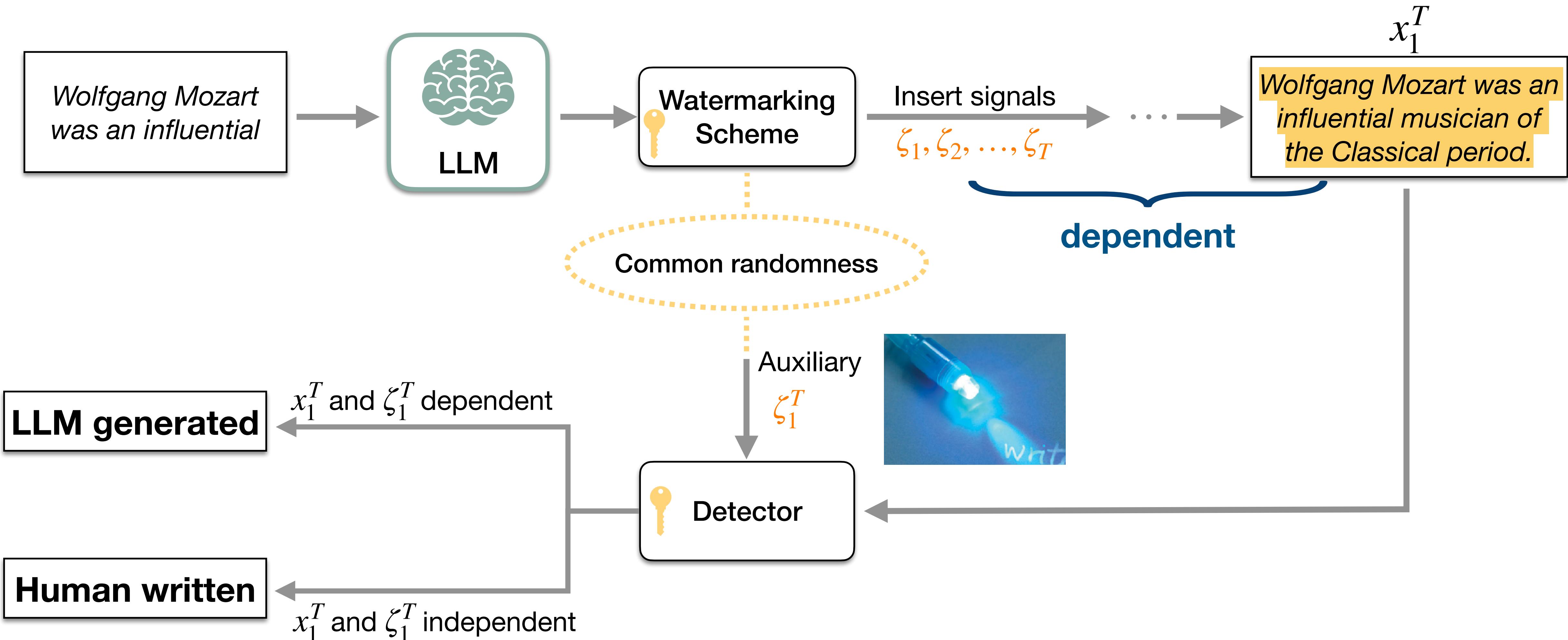
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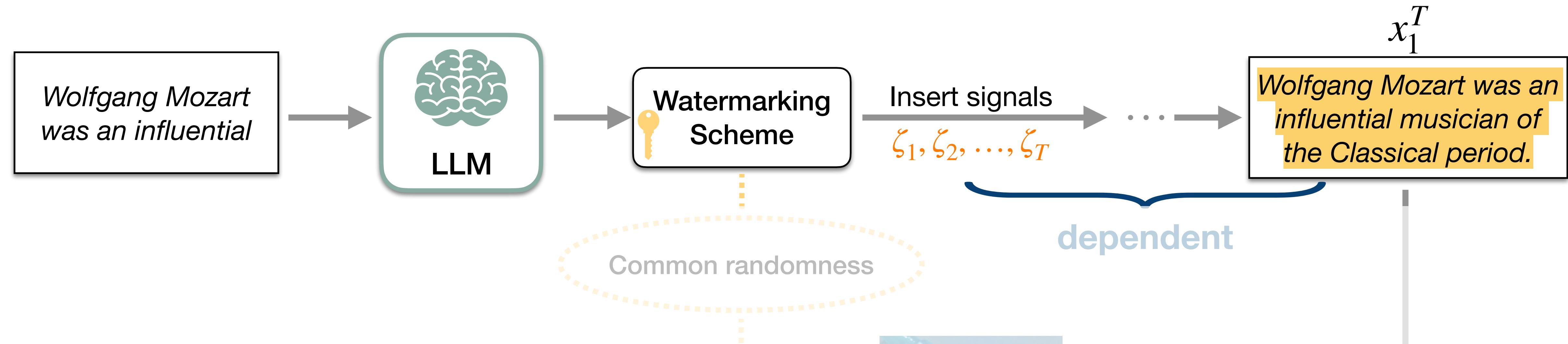
# Hypothesis Testing for LLM Watermark Detection



# Hypothesis Testing for LLM Watermark Detection



# Hypothesis Testing for LLM Watermark Detection



Watermark Detection  $\implies$  Hypothesis Testing:

$H_0 : X_1^T$  is human written, i.e.,  $(X_1^T, \zeta_1^T) \sim Q_{X_1^T} \otimes P_{\zeta_1^T}$

$H_1 : X_1^T$  is LLM generated, i.e.,  $(X_1^T, \zeta_1^T) \sim P_{X_1^T, \zeta_1^T}$

# LLM Watermark Detection Errors

Watermark Detection  $\implies$  Hypothesis Testing:

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# LLM Watermark Detection Errors

Watermark Detection  $\implies$  Hypothesis Testing: Human/unwatermarked LLM

$H_0 : X_1^T$  is human written, i.e.,  $(X_1^T, \zeta_1^T) \sim Q_{X_1^T} \otimes P_{\zeta_1^T}$

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Watermarking scheme

# LLM Watermark Detection Errors

Watermark Detection  $\implies$  Hypothesis Testing: Human/unwatermarked LLM

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Watermarking scheme

Performance metric:

# LLM Watermark Detection Errors

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Watermarking scheme

Performance metric:

Detector  $\gamma$

$$\left\{ \begin{array}{l} H_0 : \text{Human} \\ H_1 : \text{LLM} \end{array} \right.$$

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Watermarking scheme

Performance metric:

		Reality	
		$H_0$ : Human	$H_1$ : LLM
Detector $\gamma$	$H_0$ : Human		
	$H_1$ : LLM		

# LLM Watermark Detection Errors

Watermark Detection  $\implies$  Hypothesis Testing: Human/unwatermarked LLM

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Watermarking scheme

Performance metric:

		Reality	
		$H_0$ : Human	$H_1$ : LLM
Detector $\gamma$	$H_0$ : Human		
	$H_1$ : LLM	Type-I error (false alarm) $\beta_0(\gamma, Q_{X_1^T}, P_{\zeta_1^T})$	

# LLM Watermark Detection Errors

Watermark Detection  $\implies$  Hypothesis Testing: Human/unwatermarked LLM

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Watermarking scheme

Performance metric:

		Reality	
		$H_0 : \text{Human}$	$H_1 : \text{LLM}$
Detector $\gamma$	$H_0 : \text{Human}$		Type-II error (miss detection) $\beta_1(\gamma, P_{X_1^T, \zeta_1^T})$
	$H_1 : \text{LLM}$	Type-I error (false alarm) $\beta_0(\gamma, Q_{X_1^T}, P_{\zeta_1^T})$	

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Watermarking scheme

Performance metric:

		Reality	
		$H_0 : \text{Human}$	$H_1 : \text{LLM}$
Detector $\gamma$	$H_0 : \text{Human}$		Type-II error (miss detection) $\min \beta_1(\gamma, P_{X_1^T, \zeta_1^T})$
	$H_1 : \text{LLM}$	Type-I error (false alarm) $\beta_0(\gamma, Q_{X_1^T}, P_{\zeta_1^T}) \leq \alpha$	

# LLM Watermarked Text Quality

Watermark Detection  $\implies$  Hypothesis Testing: Human/unwatermarked LLM

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Watermarking scheme

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Other criteria for LLM watermarking?

scheme

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Other criteria for LLM watermarking?

$\implies$  **Text Quality!**

scheme

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Other criteria for LLM watermarking?

$\implies$  **Text Quality!**

$\implies$  **Indistinguishable from unwatermarked**

scheme

# LLM Watermarked Text Quality

Watermark Detection  $\implies$  Hypothesis Testing: Human/unwatermarked LLM

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Watermarking scheme

watermarked text distribution  
 $P_{X_1^T}$

# LLM Watermarked Text Quality

Watermark Detection  $\implies$  Hypothesis Testing: Human/unwatermarked LLM

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watermarked text distribution

$$P_{X_1^T}$$

vs

original text distribution

$$Q_{X_1^T}$$

Watermarking scheme

# LLM Watermarked Text Quality

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watermarked text distribution

$$P_{X_1^T}$$

vs

original text distribution

$$Q_{X_1^T}$$

Watermarking scheme

Good text quality

# LLM Watermarked Text Quality

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watermarked text distribution

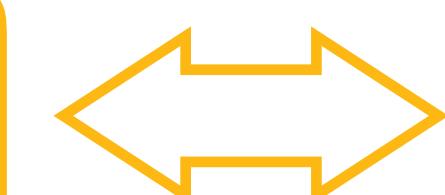
$$P_{X_1^T}$$

vs

original text distribution

$$Q_{X_1^T}$$

Good text quality



$$D(P_{X_1^T}, Q_{X_1^T}) \leq \epsilon$$

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Watermark Detection  $\implies$  Hypothesis Testing: Human/unwatermarked LLM

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watermarked text distribution

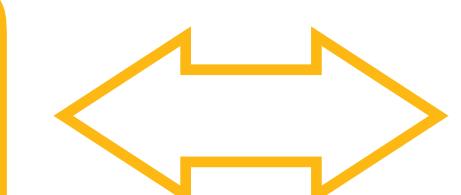
$$P_{X_1^T}$$

vs

original text distribution

$$Q_{X_1^T}$$

Good text quality



$$D(P_{X_1^T}, Q_{X_1^T}) \leq \epsilon$$

(Distortion Level)

# LLM Watermarked Text Quality

Watermark Detection  $\implies$  Hypothesis Testing: Human/unwatermarked LLM

$H_0 : X_1^T$  is human written, i.e.,  $(X_1^T, \zeta_1^T) \sim Q_{X_1^T} \otimes P_{\zeta_1^T}$

$H_1 : X_1^T$  is LLM generated, i.e.,  $(X_1^T, \zeta_1^T) \sim P_{X_1^T, \zeta_1^T}$

watermarked text distribution

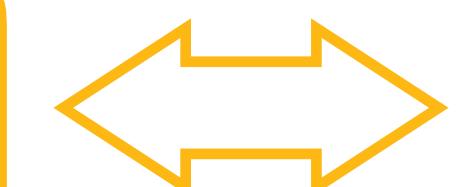
$$P_{X_1^T}$$

vs

original text distribution

$$Q_{X_1^T}$$

Good text quality



$$D(P_{X_1^T}, Q_{X_1^T}) \leq \epsilon$$

(D can be any distortion metric)

(Distortion Level)

# Trade-off in Designing LLM Watermarking

Watermark Detection  $\implies$  Hypothesis Testing: Human/unwatermarked LLM

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Watermarking scheme

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Watermarking scheme

**Trade-off:**

Type-II error — False alarm rate — Distortion Level

$$\beta_1 -- \alpha -- \epsilon$$

# Trade-off in Designing LLM Watermarking

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Existing watermarking methods: **heuristic**

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Existing watermarking methods: heuristic

Watermarking scheme

**Example**  
[KGW-1, 2023]

No watermark
Extremely efficient on average term lengths and word frequencies on synthetic, microamount text (as little as 25 words)
Very small and low-resource key/hash (e.g., 140 bits per key is sufficient for 99.99999999% of the Synthetic Internet)
With watermark
- minimal marginal probability for a detection attempt.
- Good speech frequency and energy rate reduction.
- messages indiscernible to humans.
- easy for humans to verify.

# Trade-off in Designing LLM Watermarking

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a word  $\leftarrow$  randomly assign green/red color

Green word: increase sampling probability

# Trade-off in Designing LLM Watermarking

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Existing watermarking methods: heuristic

Watermarking scheme

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Existing watermarking methods: heuristic

Watermarking scheme

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With watermark
- minimal marginal probability for a detection attempt.
- Good speech frequency and energy rate reduction.
- messages indiscernible to humans.
- easy for humans to verify.

- High miss detection when requiring low false alarm
- Not distortion-free

# Optimize LLM Watermark Generation and Detection

Watermark Detection  $\implies$  Hypothesis Testing: Human/unwatermarked LLM

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Watermarking scheme

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Find the best watermarking scheme & detector:

Watermarking scheme

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Find the best watermarking scheme & detector:

Minimize miss detection

$$\min_{\gamma, P_{X_1^T, \zeta_1^T}} \beta_1(\gamma, P_{X_1^T, \zeta_1^T})$$

Watermarking scheme

# Optimize LLM Watermark Generation and Detection

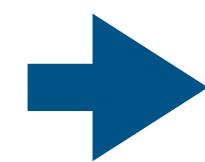
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Humans are very creative,  
can write arbitrary texts



Watermarking scheme

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Humans are very creative,  
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Watermarking scheme

# Optimize LLM Watermark Generation and Detection

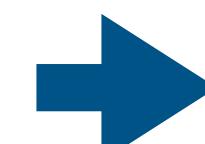
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Ensure text quality



Watermarking scheme

# Optimize LLM Watermark Generation and Detection

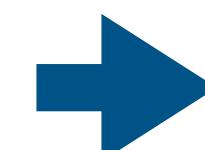
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Ensure text quality



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Watermarking scheme

# Fundamental Limit for Type-II Error

**Optimization problem:**

$$\min_{\gamma, P_{X_1^T, \zeta_1^T}} \beta_1(\gamma, P_{X_1^T, \zeta_1^T})$$

$$\text{s.t. } \sup_{Q_{X_1^T}} \beta_0(\gamma, Q_{X_1^T}, P_{\zeta_1^T}) \leq \alpha$$

$$D(P_{X_1^T}, Q_{X_1^T}) \leq \epsilon$$

# Fundamental Limit for Type-II Error

Watermarked text distribution:

$$P_{X_1^T}^* = \arg \min_{P_{X_1^T}: D(P_{X_1^T}, Q_{X_1^T}) \leq \epsilon} \sum_{x_1^T} (P_{X_1^T}(x_1^T) - \alpha)_+$$

## Optimization problem:

$$\min_{\gamma, P_{X_1^T, \zeta_1^T}} \beta_1(\gamma, P_{X_1^T, \zeta_1^T})$$

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## ◆ Minimum Type-II error:

$$\beta_1^*(Q_{X_1^T}, \alpha, \epsilon) = \sum_{x_1^T} (P_{X_1^T}^*(x_1^T) - \alpha)_+$$

# Fundamental Limit for Type-II Error

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$$D(P_{X_1^T}, Q_{X_1^T}) \leq \epsilon$$

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$$\beta_1^*(Q_{X_1^T}, \alpha, \epsilon) = \sum_{x_1^T} (P_{X_1^T}^*(x_1^T) - \alpha)_+$$

**Best achievable for any  
watermarking methods**

Same as Huang et al. (2023, Theorem 3.2)  
but under different framework

# Fundamental Limit for Type-II Error

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$D_{TV}$

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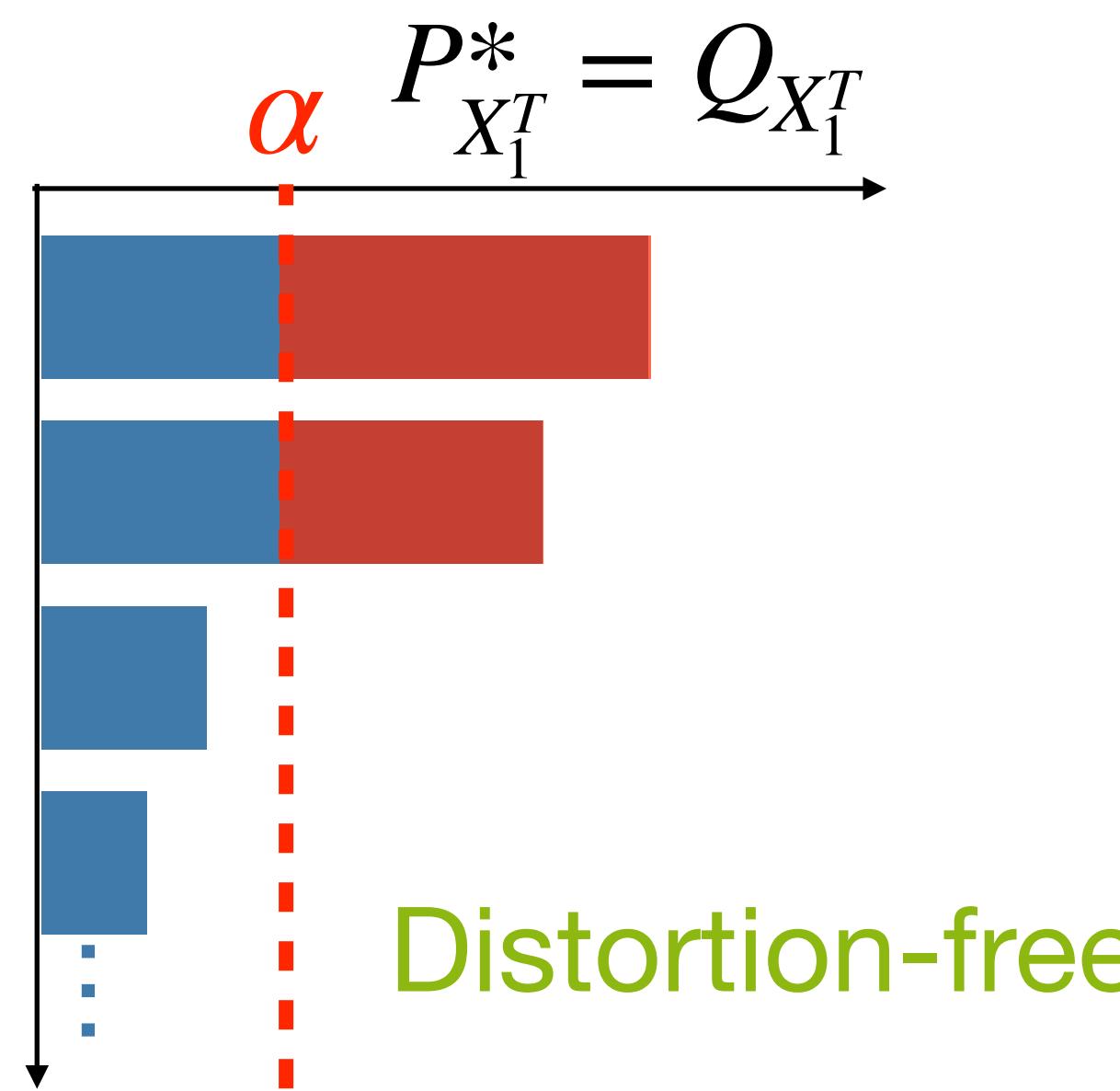
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$$\beta_1^*(Q_{X_1^T}, \alpha, \epsilon) = \sum_{x_1^T} (P_{X_1^T}^*(x_1^T) - \alpha)_+$$



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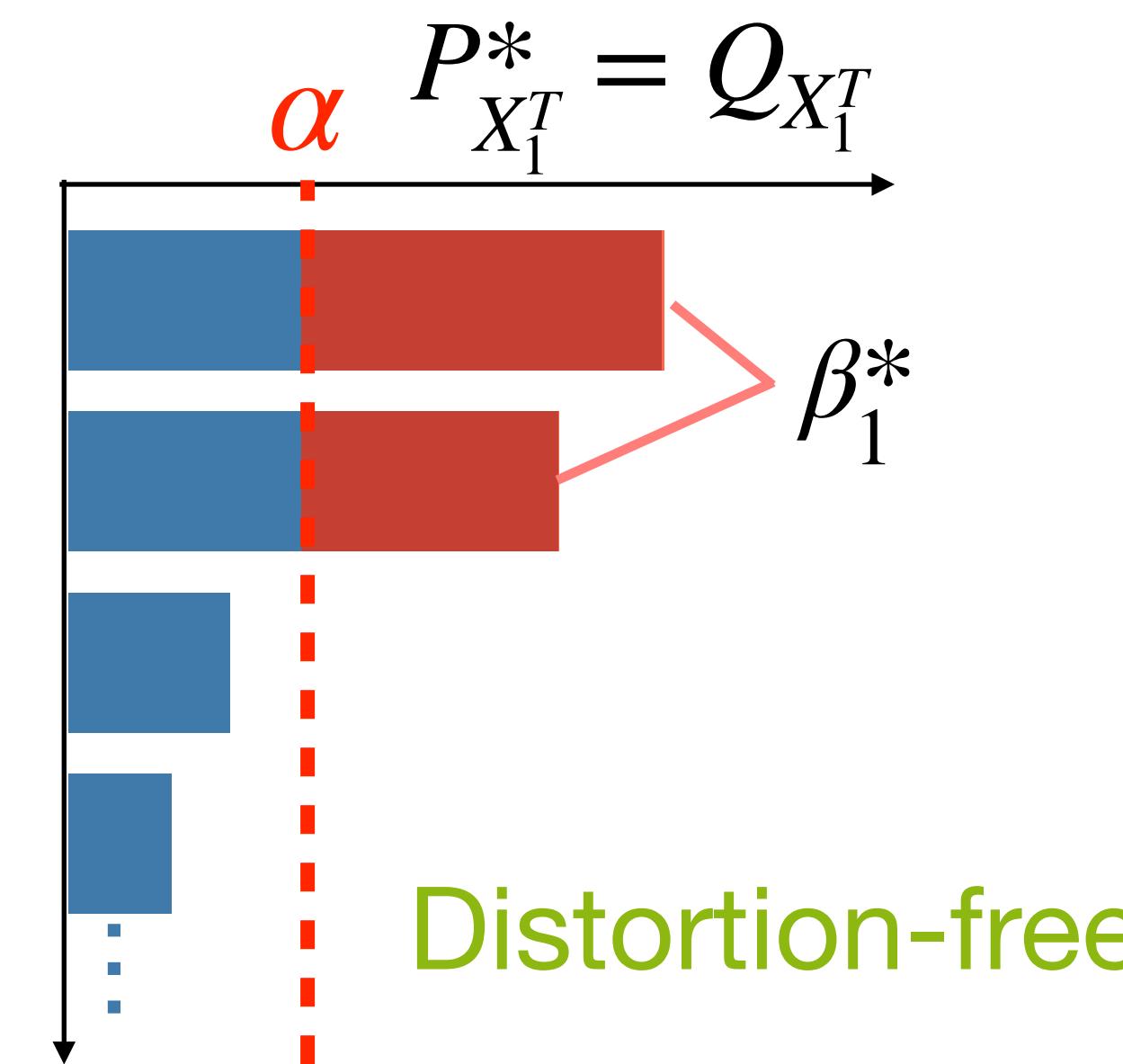
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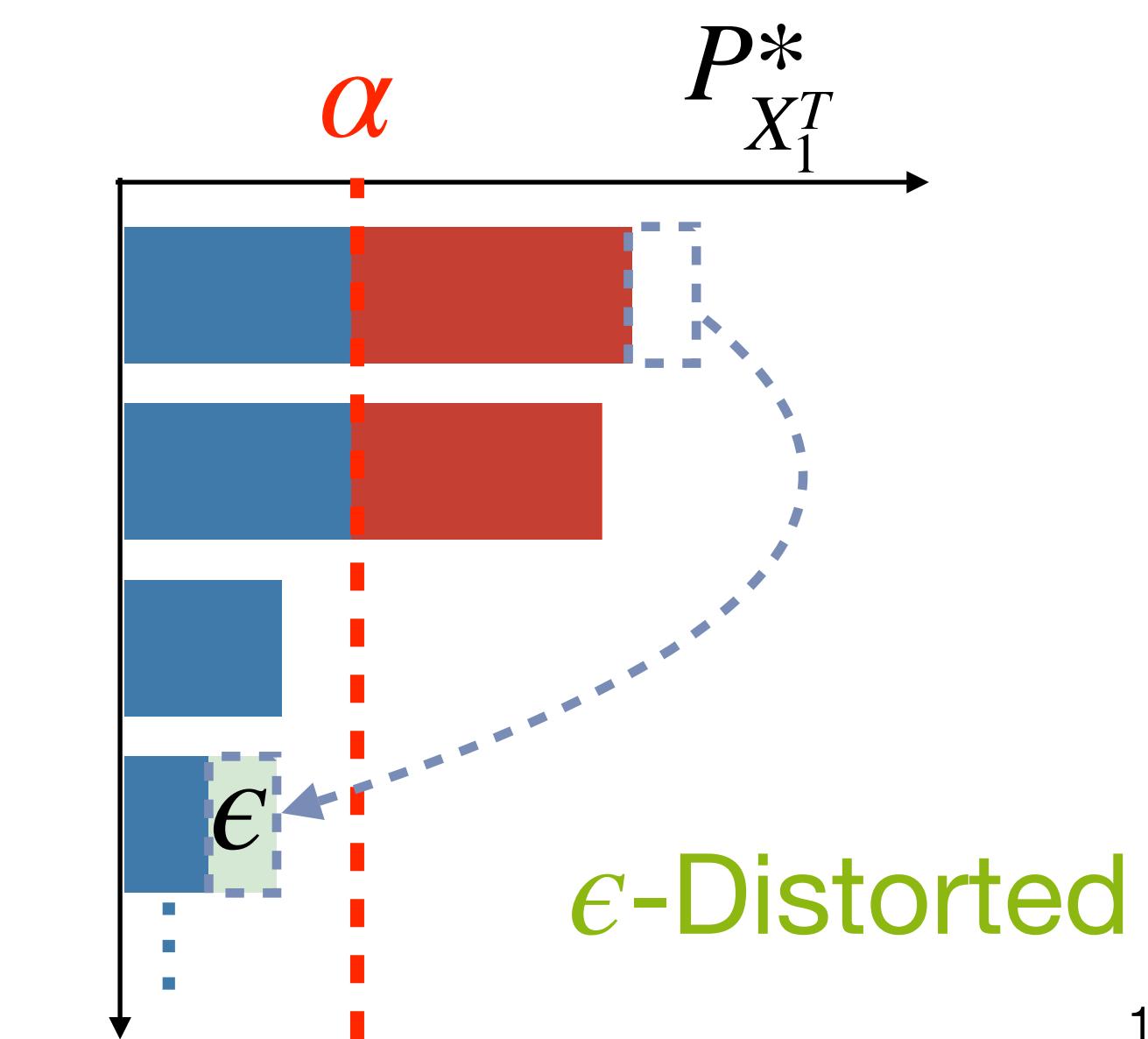
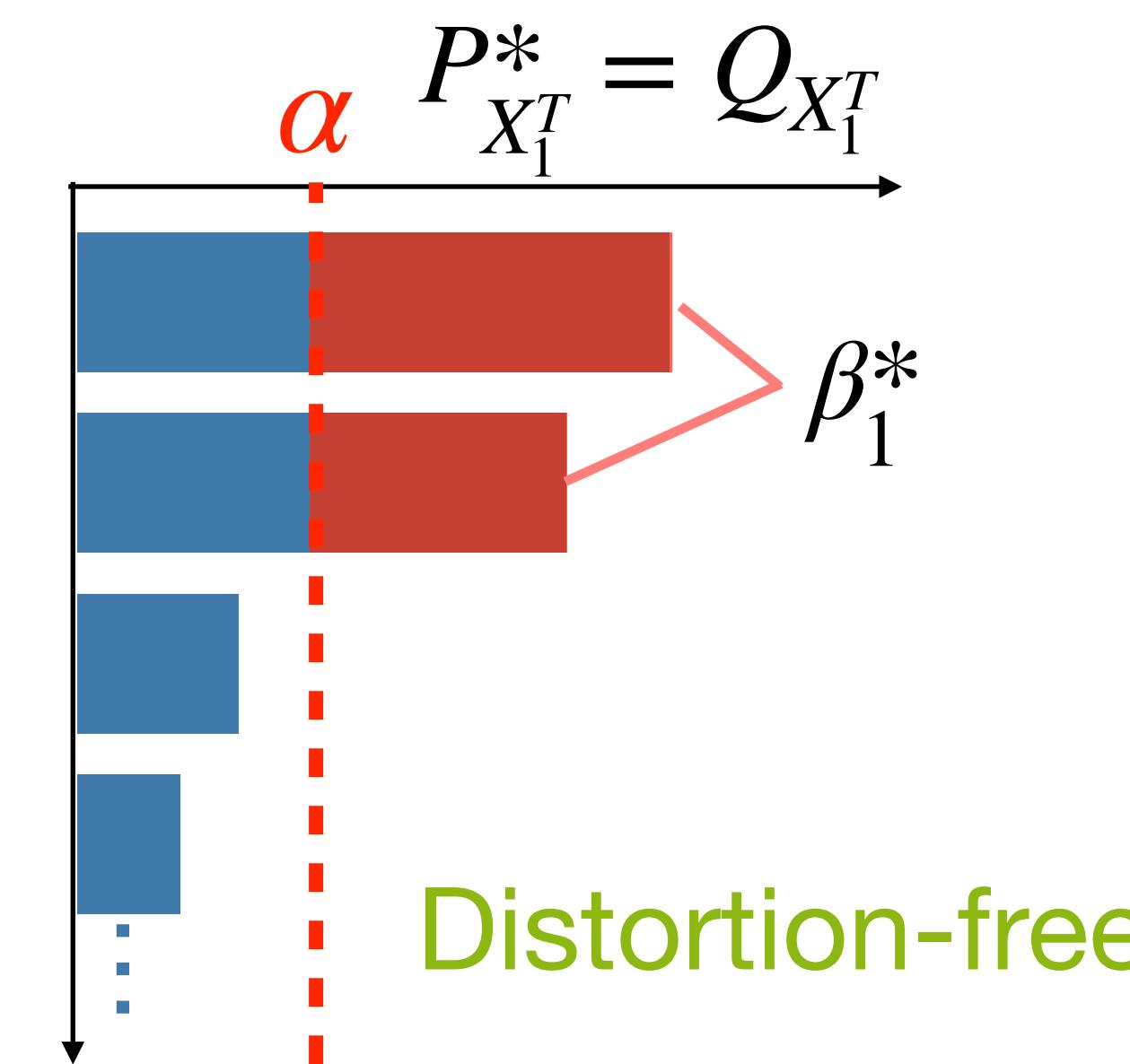
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$$D(P_{X_1^T}, Q_{X_1^T}) \leq \epsilon$$

$$D_{TV}$$

## ◆ Minimum Type-II error:

$$\beta_1^*(Q_{X_1^T}, \alpha, \epsilon) = \sum_{x_1^T} (P_{X_1^T}^*(x_1^T) - \alpha)_+$$



# Fundamental Limit for Type-II Error

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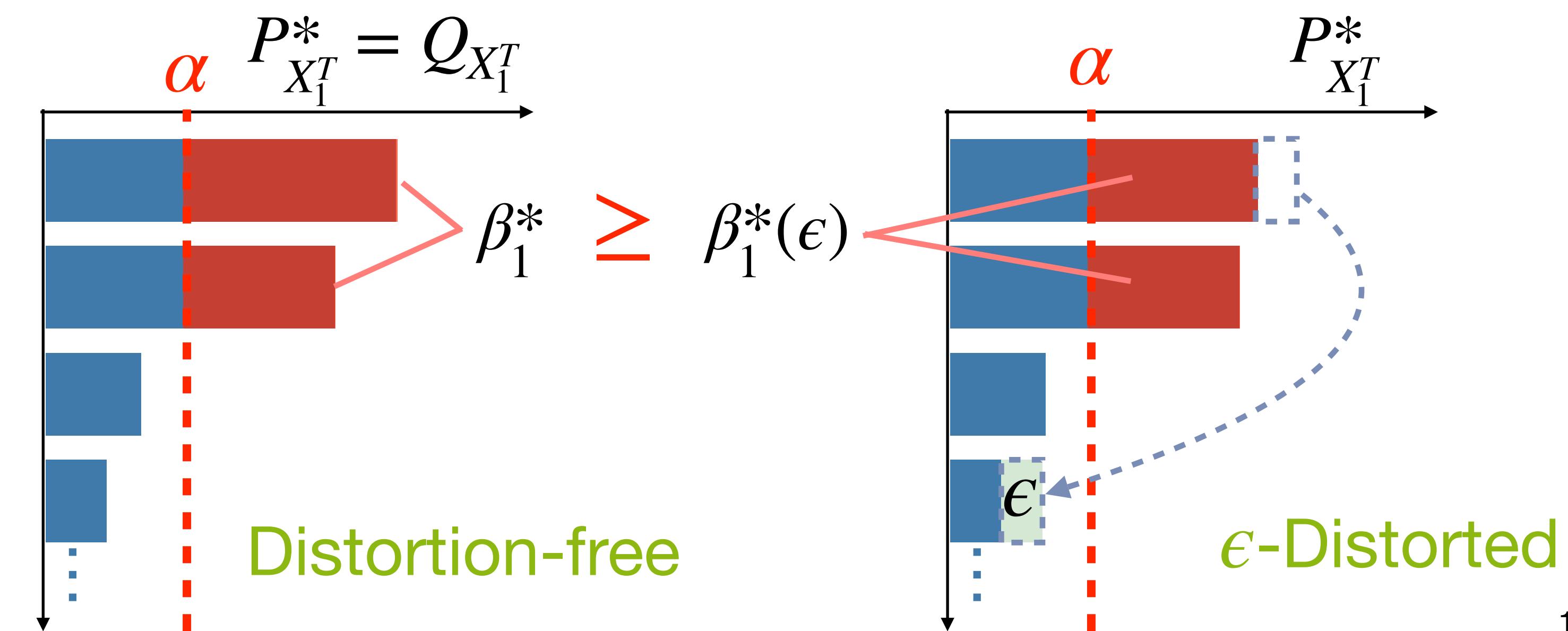
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$D_{TV}$

## ◆ Minimum Type-II error:

$$\beta_1^*(Q_{X_1^T}, \alpha, \epsilon) = \sum_{x_1^T} (P_{X_1^T}^*(x_1^T) - \alpha)_+$$



# Jointly Optimal Detector and Watermarking Scheme

**Optimization problem:**

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# Jointly Optimal Detector and Watermarking Scheme

◆ Jointly optimal detector  $\gamma^*$  and watermarking scheme  $P_{X_1^T, \zeta_1^T}^*$ :

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Optimization problem:

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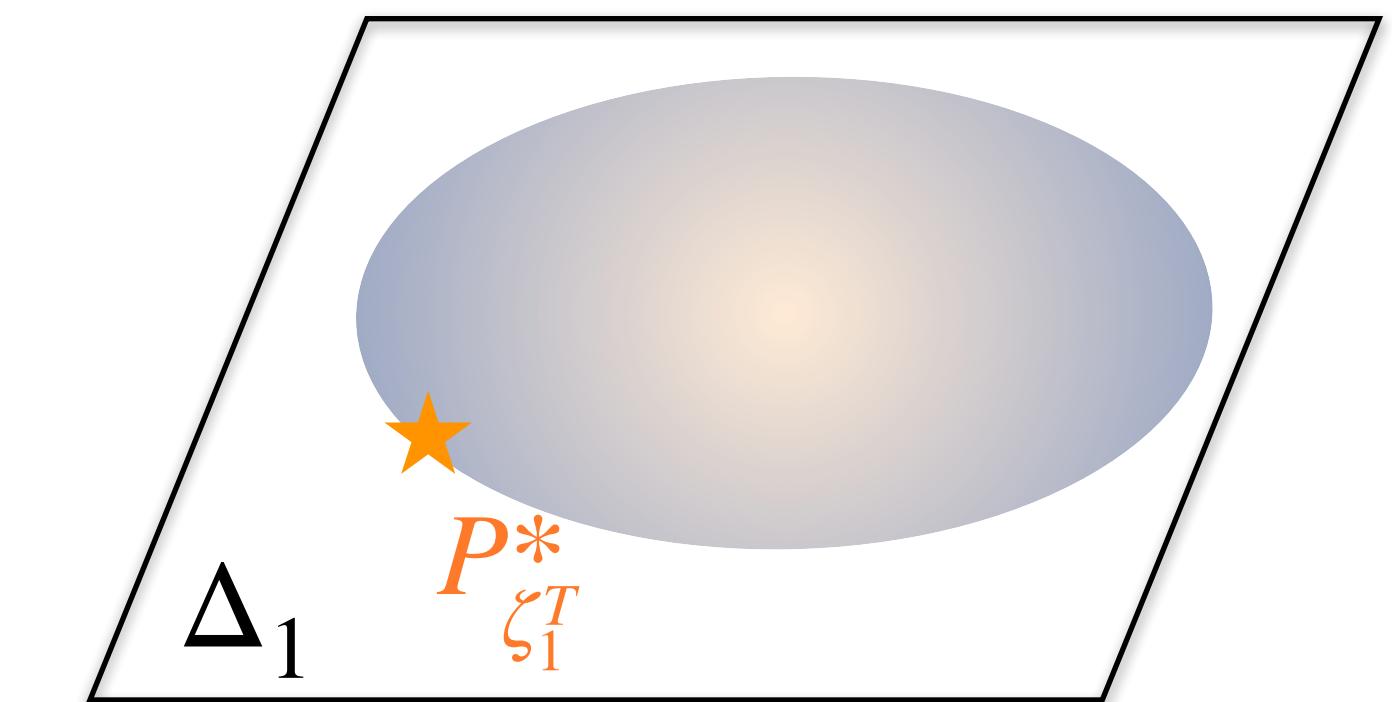
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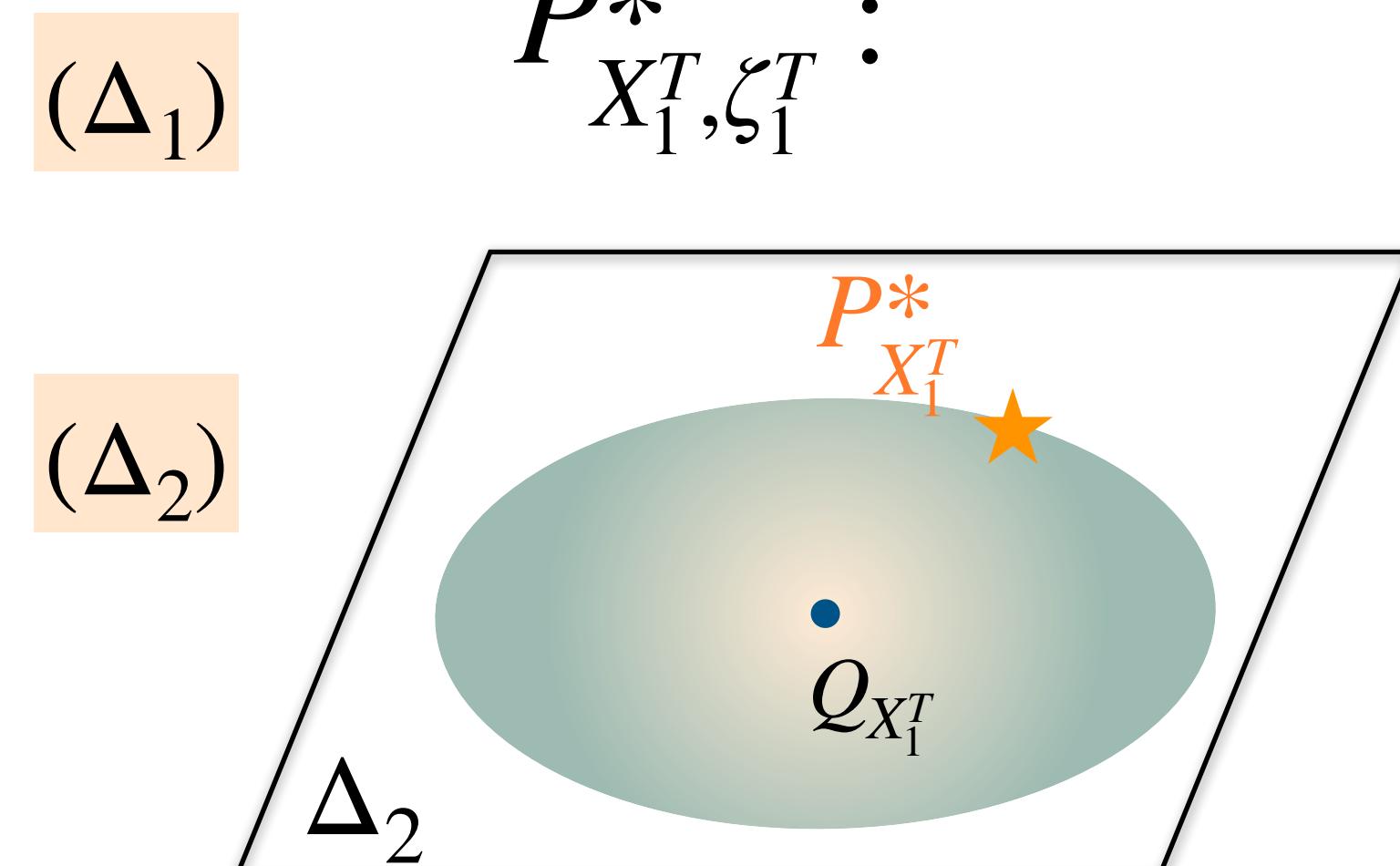
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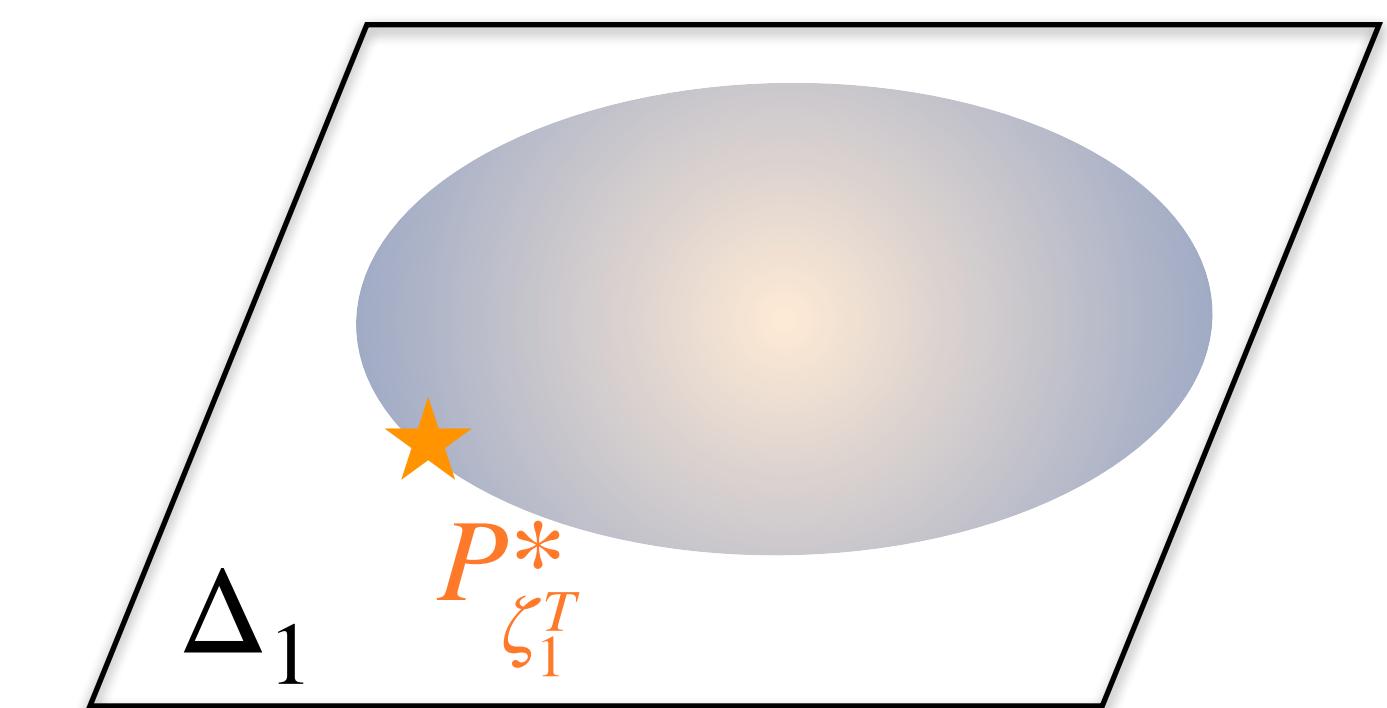
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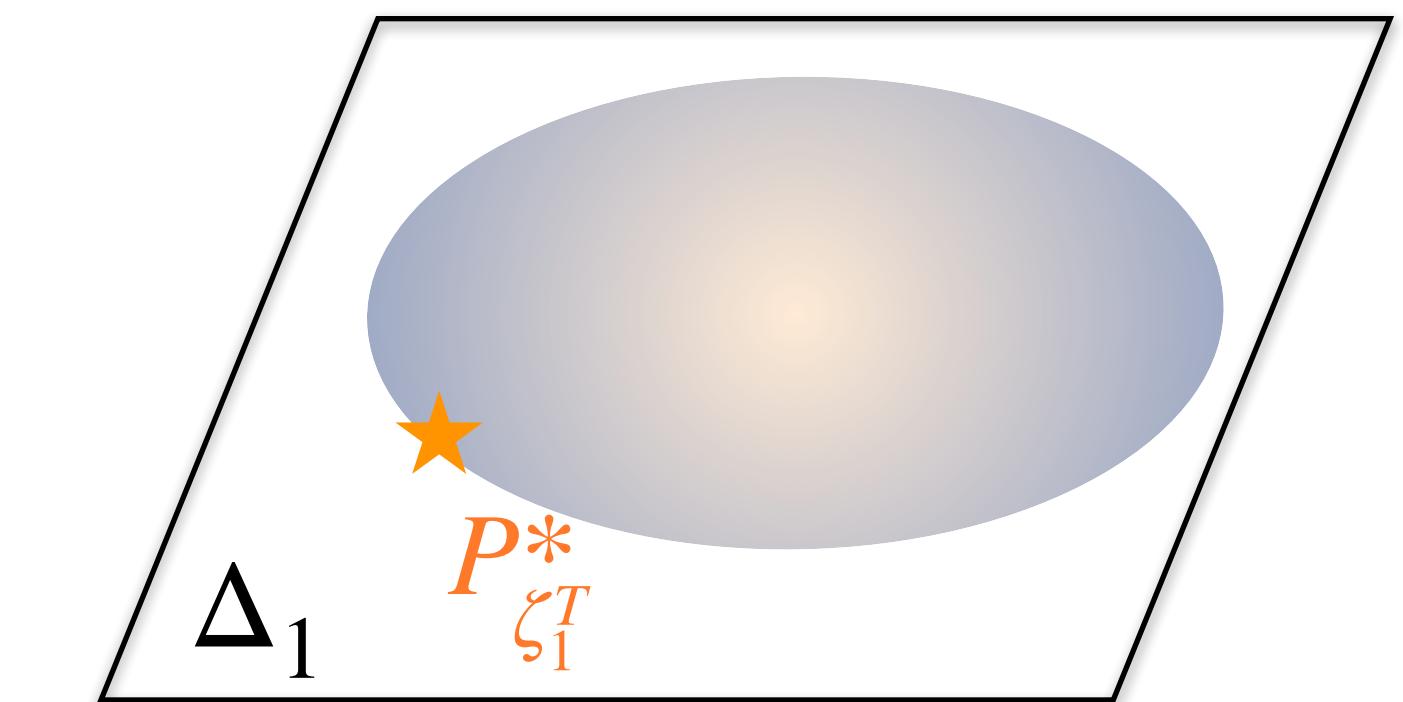
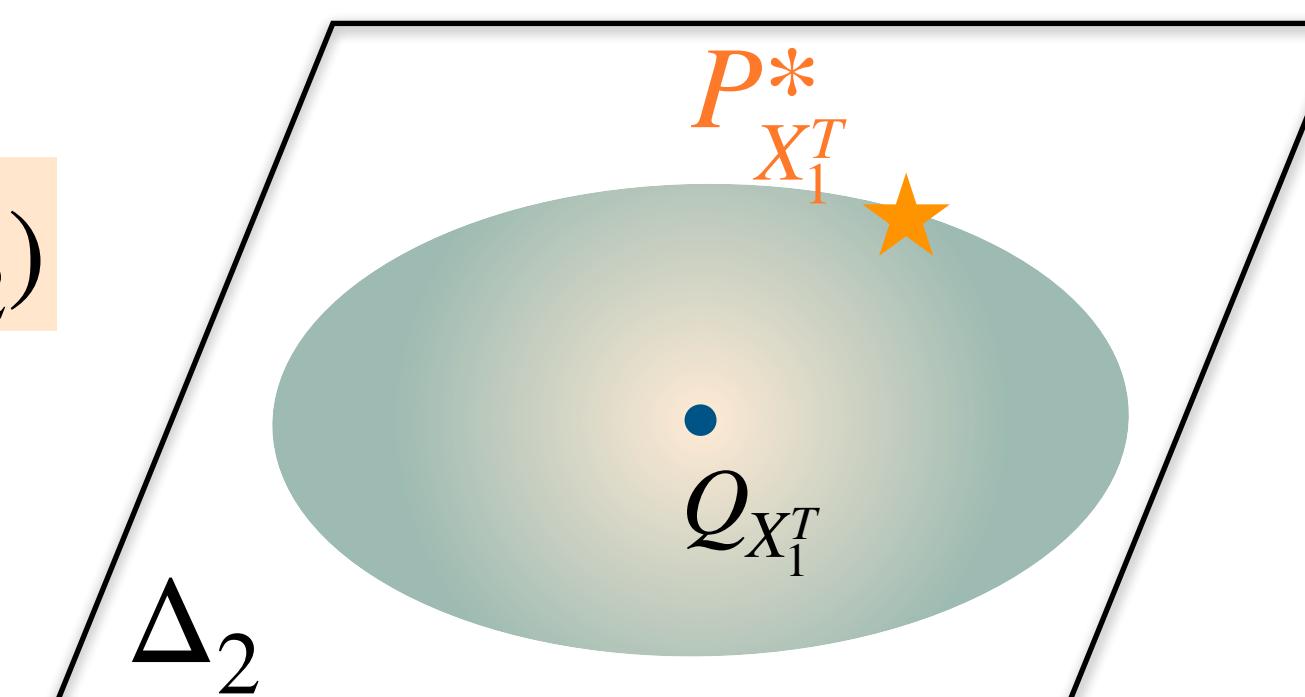
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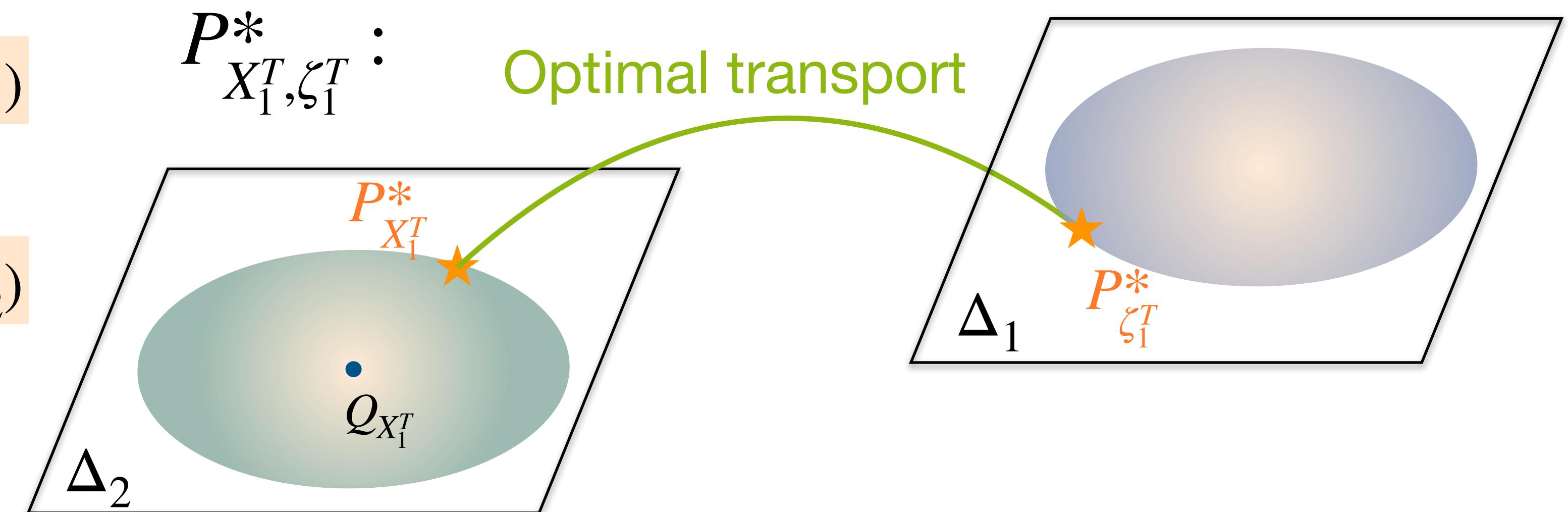
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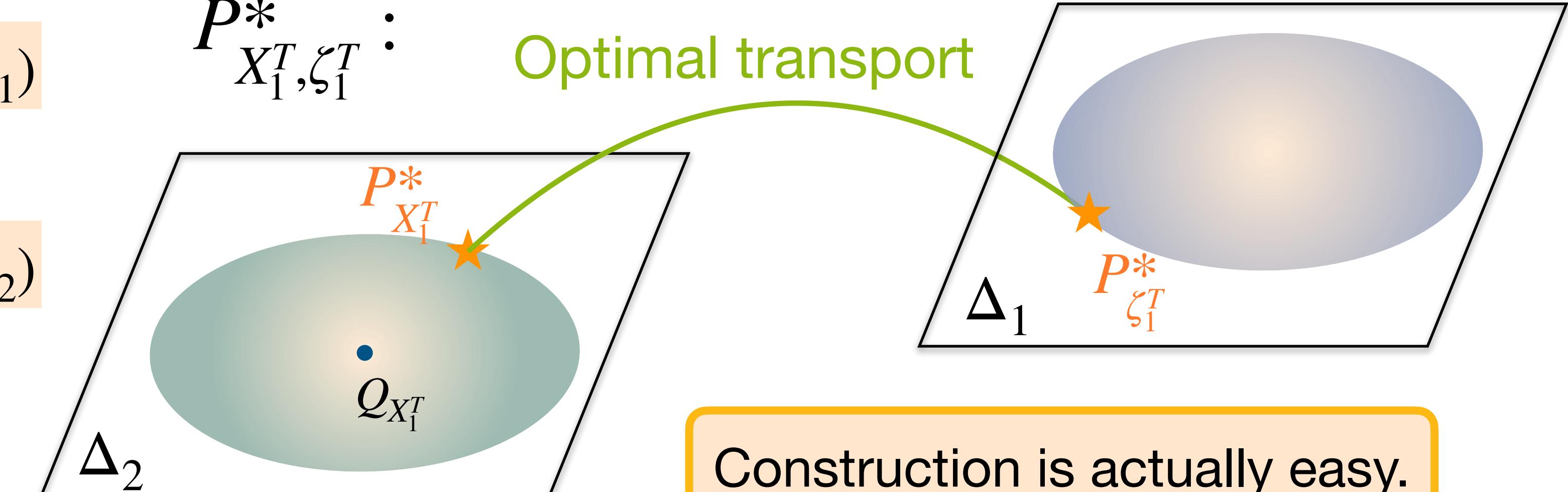
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Optimal transport



Construction is actually easy.

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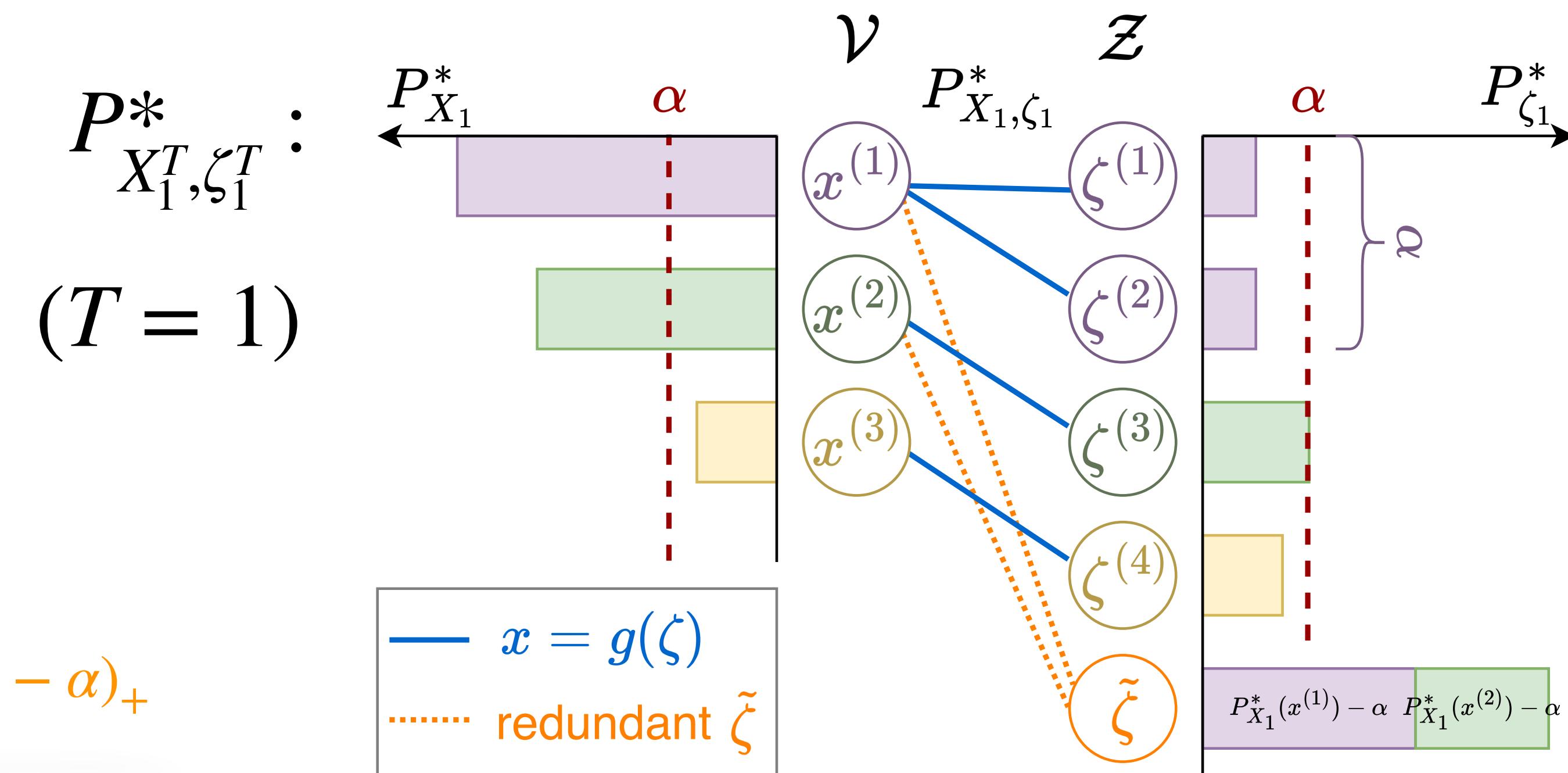
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Unlike existing watermarking methods

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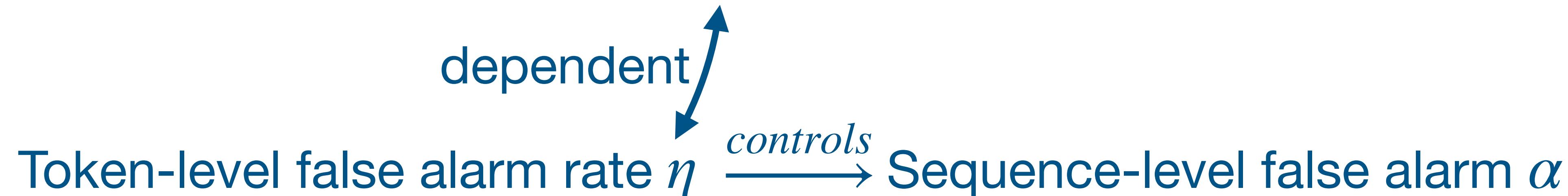
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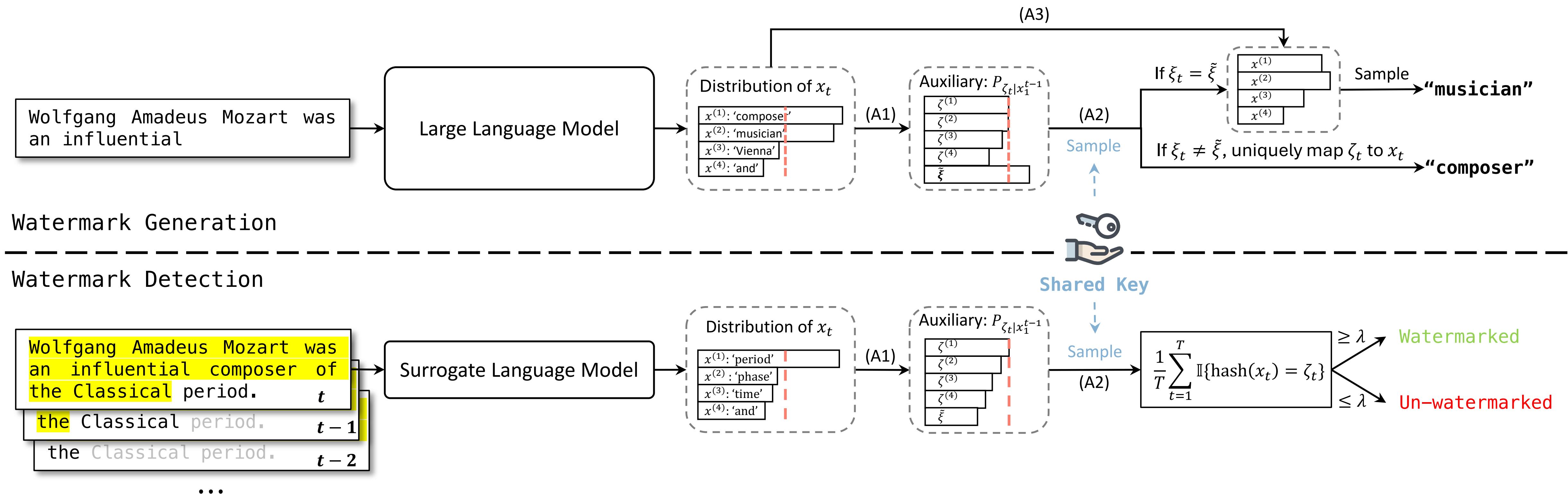
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# DAWA: Distribution-Adaptive Watermarking Algorithm

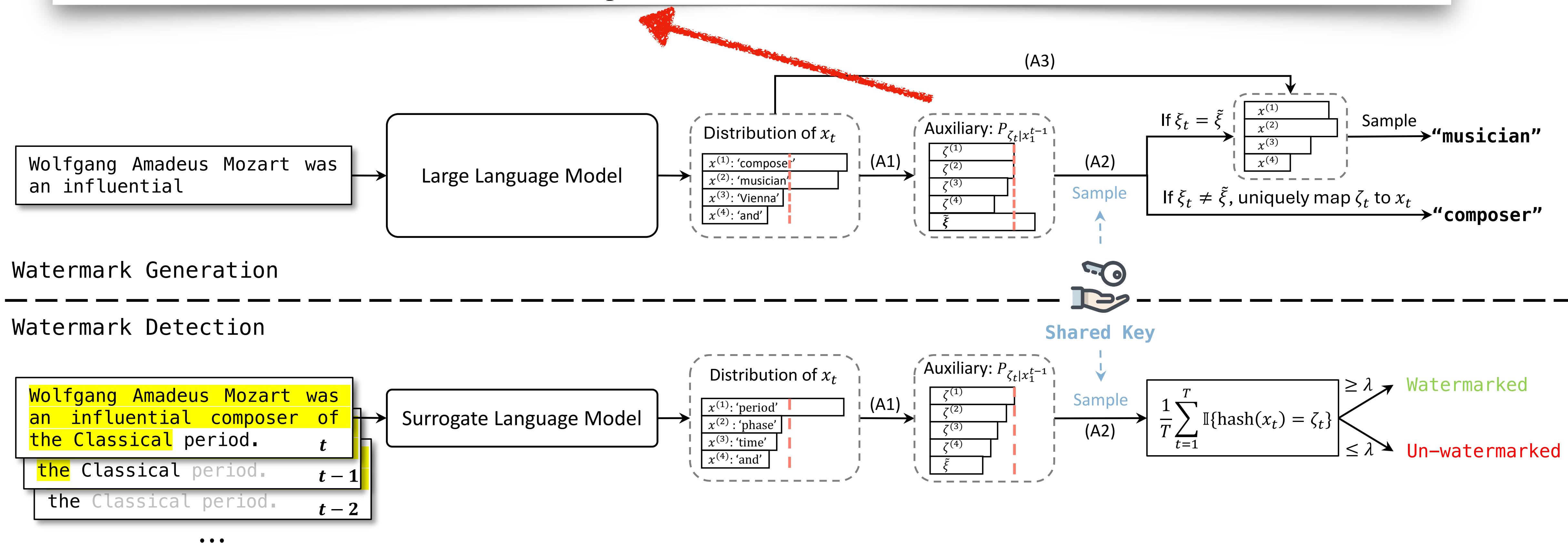
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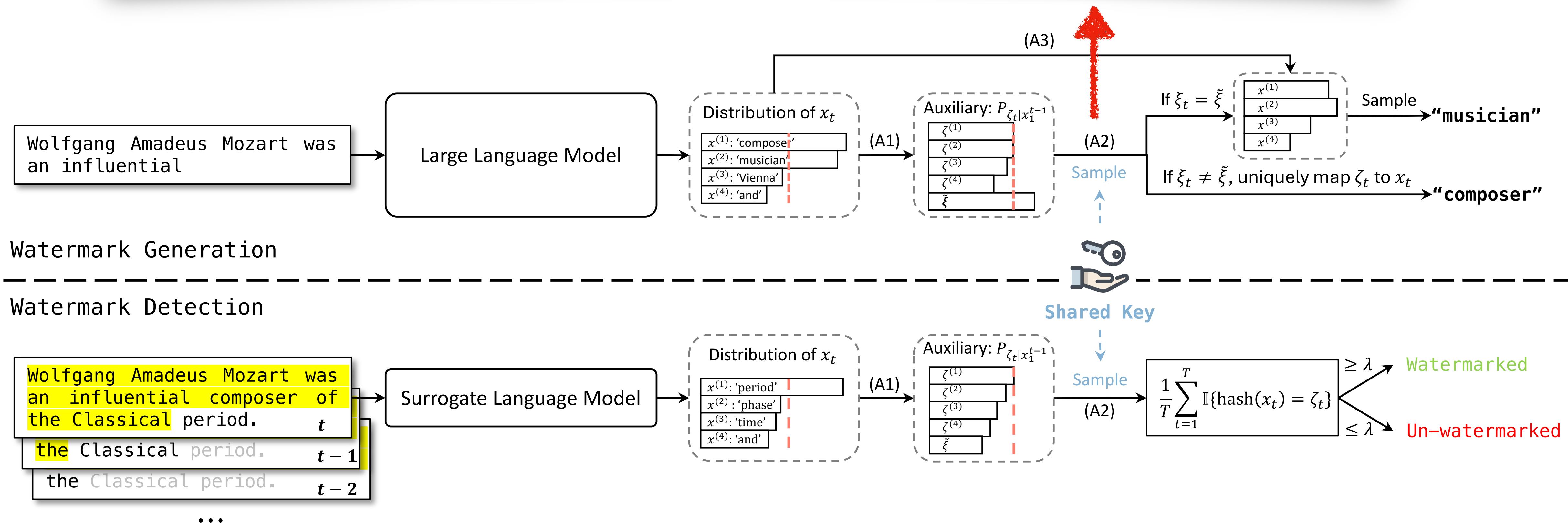
At each time  $t$ , construct  $P_{\zeta_t|X_1^t}^*$  from the LLM predicted distribution  $Q_{X_t|X_1^{t-1}}$



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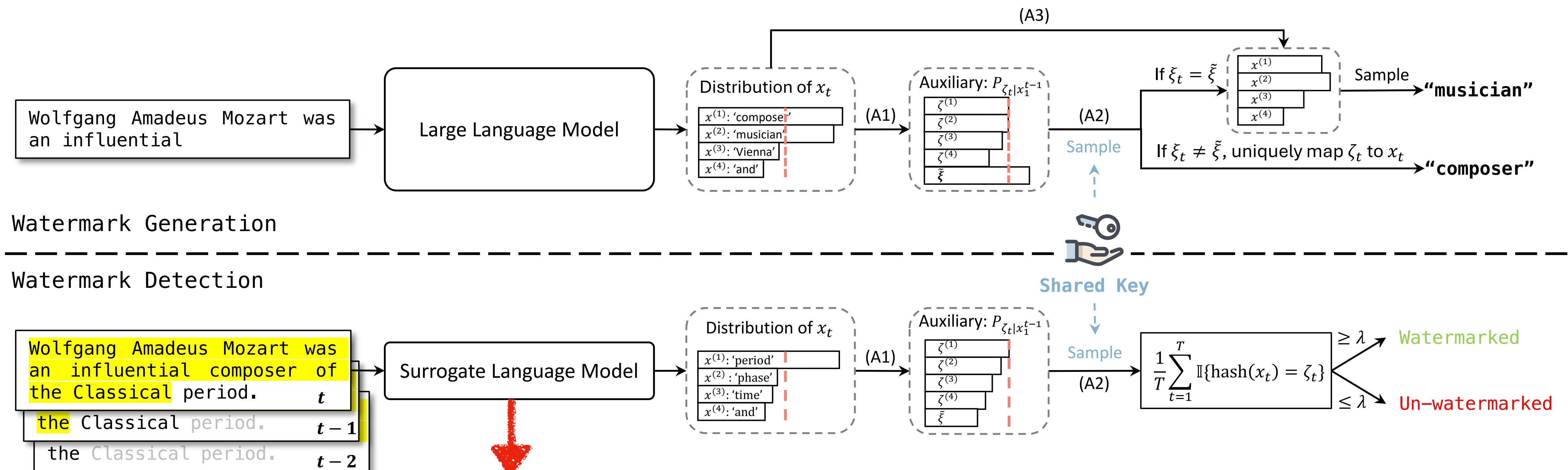
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Sample  $\zeta_t$  using Gumbel max trick:  $\zeta_t \leftarrow \arg \max_{\zeta} \log P_{\zeta_t|x_1^t}^*(\zeta) + G_{\zeta,t}$



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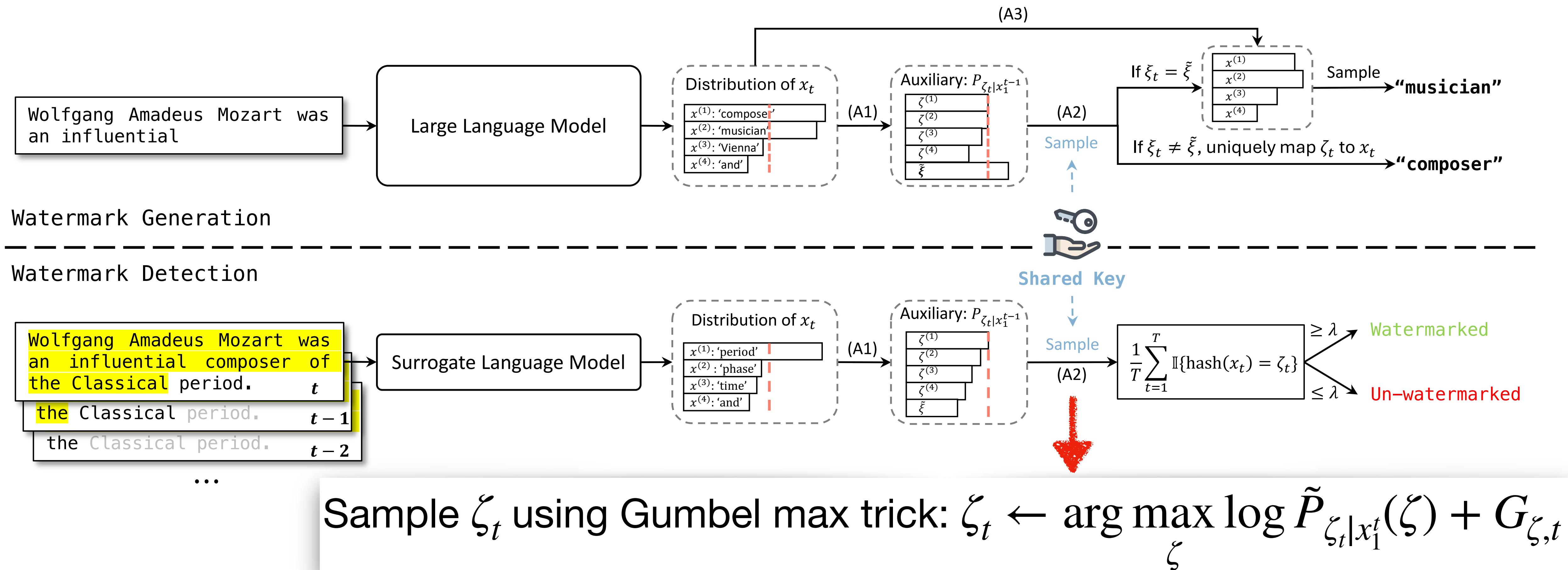
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Approximate distribution of  $X_t$  so as to construct  $\tilde{P}_{\zeta_t|x_1^{t-1}}$

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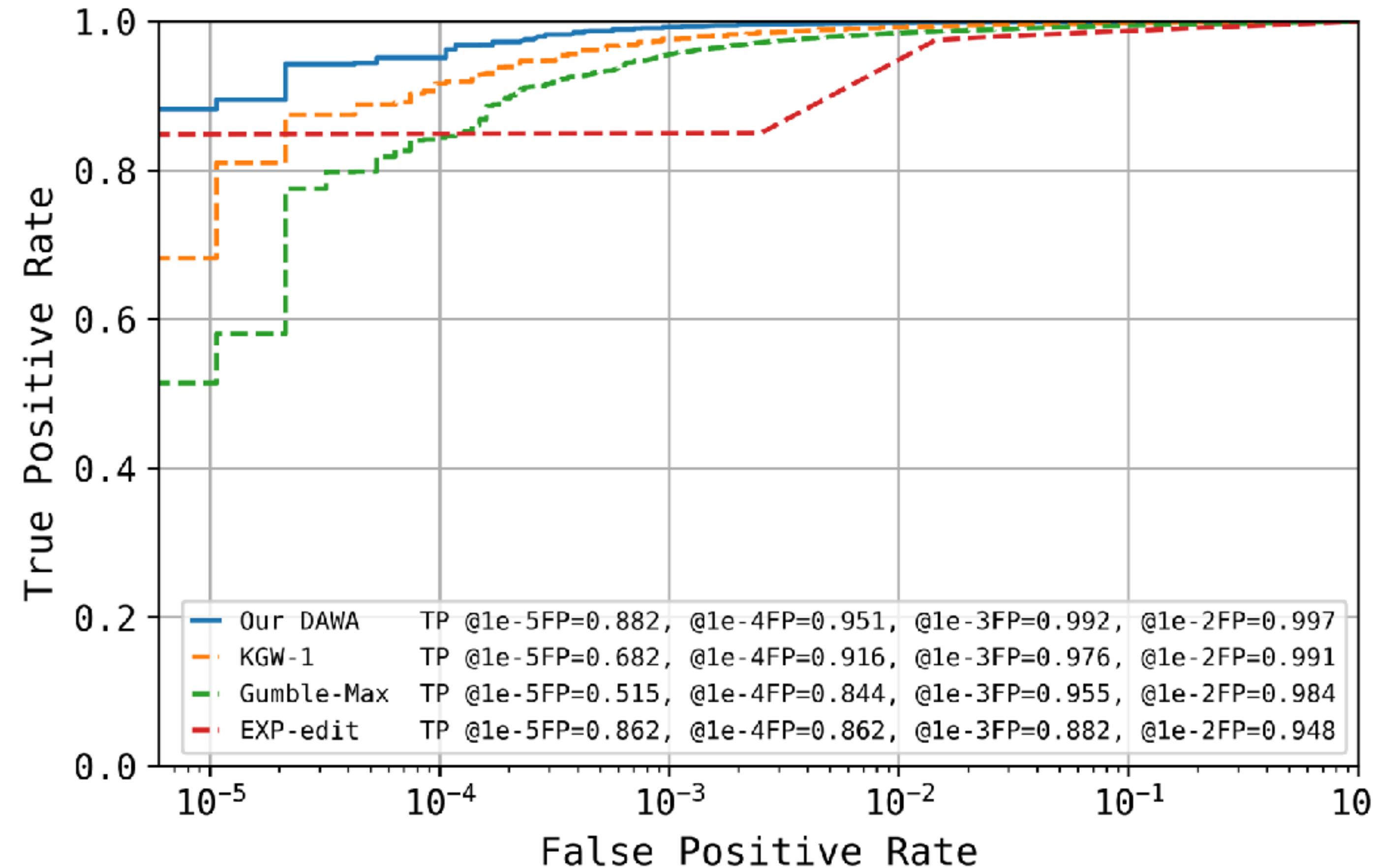
# Experimental Result

**DAWA (Distribution-Adaptive Watermarking Algorithm)**

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## DAWA (Distribution-Adaptive Watermarking Algorithm)

Fast and  
Accurate



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## DAWA (Distribution-Adaptive Watermarking Algorithm)

Fast and  
Accurate

Text quality  
high



Methods	Human	KGW-1	EXP-Edit	Gumbel-Max	Ours
BLEU Score	0.219	0.158	0.203	0.210	0.214
Avg Perplexity	8.846	14.327	12.186	11.732	6.495

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# Robustness Against Text Modifications

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$$D(P_{X_1^T}, Q_{X_1^T}) \leq \epsilon$$

♦ Minimum  $f$ -robust Type-II error:

$$\begin{aligned} \beta_1^*(Q_{X_1^T}, \alpha, \epsilon, f) \\ = \min_{P_{X_1^T}: D(P_{X_1^T}, Q_{X_1^T}) \leq \epsilon} \sum_{k \in [K]} \left( \left( \sum_{x_1^T: f(x_1^T)=k} P_{X_1^T}(x_1^T) \right) - \alpha \right)_+ \end{aligned}$$

# Robustness Against Text Modifications

Optimization problem:

$$\begin{aligned} \min_{\gamma, P_{X_1^T, \zeta_1^T}} \quad & \beta_1(\gamma, P_{X_1^T, \zeta_1^T}, f) \\ \text{s.t.} \quad & \sup_{Q_{X_1^T}} \beta_0(\gamma, Q_{X_1^T}, P_{\zeta_1^T}, f) \leq \alpha \\ & D(P_{X_1^T}, Q_{X_1^T}) \leq \epsilon \end{aligned}$$

♦ Minimum  $f$ -robust Type-II error:

$$\begin{aligned} \beta_1^*(Q_{X_1^T}, \alpha, \epsilon, f) \\ = \min_{P_{X_1^T}: D(P_{X_1^T}, Q_{X_1^T}) \leq \epsilon} \sum_{k \in [K]} \left( \left( \sum_{x_1^T: f(x_1^T)=k} P_{X_1^T}(x_1^T) \right) - \alpha \right)_+ \end{aligned}$$

Higher than the minimum Type-II error  
without considering robustness

# Robustness Against Text Modifications

Optimization problem:

$$\begin{aligned} \min_{\gamma, P_{X_1^T, \zeta_1^T}} \quad & \beta_1(\gamma, P_{X_1^T, \zeta_1^T}, f) \\ \text{s.t.} \quad & \sup_{Q_{X_1^T}} \beta_0(\gamma, Q_{X_1^T}, P_{\zeta_1^T}, f) \leq \alpha \\ & D(P_{X_1^T}, Q_{X_1^T}) \leq \epsilon \end{aligned}$$

♦ Minimum  $f$ -robust Type-II error:

$$\begin{aligned} \beta_1^*(Q_{X_1^T}, \alpha, \epsilon, f) \\ = \min_{P_{X_1^T}: D(P_{X_1^T}, Q_{X_1^T}) \leq \epsilon} \sum_{k \in [K]} \left( \left( \sum_{x_1^T: f(x_1^T)=k} P_{X_1^T}(x_1^T) \right) - \alpha \right)_+ \end{aligned}$$

Higher than the minimum Type-II error  
without considering robustness

♦ Optimal watermarking scheme:

add signal  $\zeta_1^T$  to  $P_{f(X_1^T)}$ , e.g., in the semantic space