LLM Training and Coding for Statistical Learning and Data Science

Part 2: API Usage and Text Watermarking

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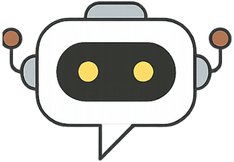
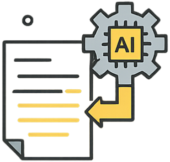
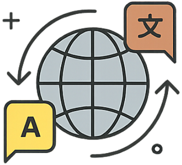
LLMs in everyday use



Chatbots

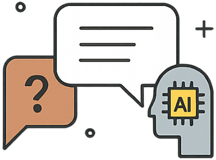


Text generration

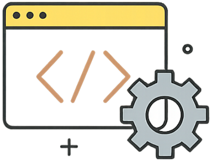


Language translation

Sentiment analysis



Question answering



Code generation

Bringing LLMs into everyday applications

- ChatGPT and other LLMs are powerful, but web interfaces limit automation.
- To integrate LLMs into software, we use an **API** (Application Programming Interface).
- APIs let developers send text prompts and receive model-generated responses.
- Conceptually, an API treats the LLM as a **black box** that returns outputs in a **function-calling** manner.
- This enables customized assistants, summarizers, or analytic tools.

Applications built on the ChatGPT API

- **Chatbots and Assistants:** Integrations like Notion AI and Instacart's shopping assistant use the API to answer user queries and automate workflows.
- **Content and Writing Tools:** Tools such as Jasper and Copy.ai use the API for marketing text, article generation, and idea expansion.
- **Developer Tools:** Examples include GitHub Copilot for code suggestions and various OpenAI project demos for SQL translation or tutoring.
- **Summarization and Knowledge Extraction:** Apps like Yext use the API to build domain-specific QA systems from large document sets.
- **Specialized Research and Healthcare:** For instance, researchers have used the API to aid in systematic clinical review screening.

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API is not everything

The ChatGPT API acts as a reasoning engine: it generates intelligent responses, while the whole application handles more things such as context, interaction, and control.

Getting started with the ChatGPT API

1. Create an OpenAI account via `auth.openai.com/create-account`.
2. **Get your API key** via `platform.openai.com/account/api-keys`.

NAME	SECRET KEY	LAST USED ⓘ	CREATED BY	PERMISSIONS
Secret key	sk-...2GQA	Never	Xiang Li	All

3. Store the API key securely (as an environment variable or in a secret manager).
4. Install the client library, e.g.:
    - `pip install openai`
5. Start querying the model!

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Cost of APIs

Using the API is billed per token: e.g., GPT-5 mini currently costs about \$0.25 per 1 M input tokens and \$2 per 1 M output tokens (see official pricing).

Minimal Python Example

Goal: send a user message and get a response.

```python
from openai import OpenAI
client = OpenAI(api_key="your_api_key_here")

resp = client.chat.completions.create(
    model="gpt-4o-mini",
    messages=[
        {"role": "system", "content": "You are a helpful assistant."},
        {"role": "user", "content": "Explain PCA in 3 short bullets."}
        ]
)

answer = resp.choices[0].message.content
```

Model Output Example

Model output:

```
- **Dimensionality Reduction**: Principal Component Analysis (PCA) transforms high-dimensional data into a lower-dimensional space while preserving as much variance (information) as possible.

- **Orthogonal Transformation**: It achieves this by identifying new axes (principal components) that are linear combinations of the original features, where each principal component is orthogonal to one another.

- **Variance Maximization**: The first principal component captures the direction of the greatest variance in the data, and subsequent components capture the remaining variance in orthogonal directions.
```

Tuning Model Parameters in the ChatGPT API

The API provides flexible parameters to control generation behavior. See https://platform.openai.com/docs/api-reference/completions for more.

Key parameters:

- `temperature` – randomness of responses ($0 =$ deterministic, $1 =$ creative)
- `max_tokens` – limit on output length
- `top_p` – nucleus sampling [Holtzman et al., 2020], top-p probability mass
- `frequency_penalty` – discourages repetition of frequent tokens
- `presence_penalty` – encourages introducing new topics

```
resp = client.chat.completions.create(
    model="gpt-4o-mini",
    temperature=0.8,
    max_tokens=200,
    top_p=0.9,
    frequency_penalty=0.2,
    presence_penalty=0.6,
    messages=[......])
```

Beyond chat: Other OpenAI API capabilities

The API supports many tasks beyond text generation.

- **Embeddings & Search:** Convert text to vector form for similarity, clustering, or retrieval.
- **Multimodal Input:** Process or generate images (e.g., analysis, editing, or description).
- **Function Calling:** Let models call external tools or return structured JSON outputs.
- **Reasoning Tasks:** Use models with better step-by-step reasoning ability.
- **Fine-tuning:** Train models on domain-specific data to match your tone or tasks.

Check `https://platform.openai.com/docs/api-reference` for more details.

An example: Model evaluation via APIs

- Even with only API access, we can still conduct meaningful statistical research.
- APIs provide access to LLM intelligence, but interpreting their behavior and improving their utility require statistical thinking.
- For example, suppose we want to evaluate how many theorems an LLM knows.

An example: Model evaluation via APIs

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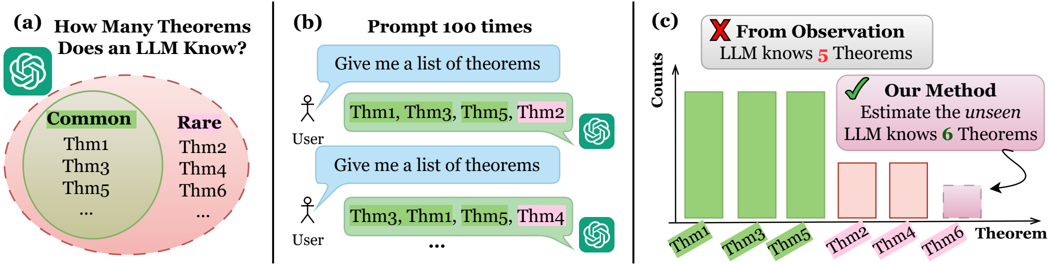
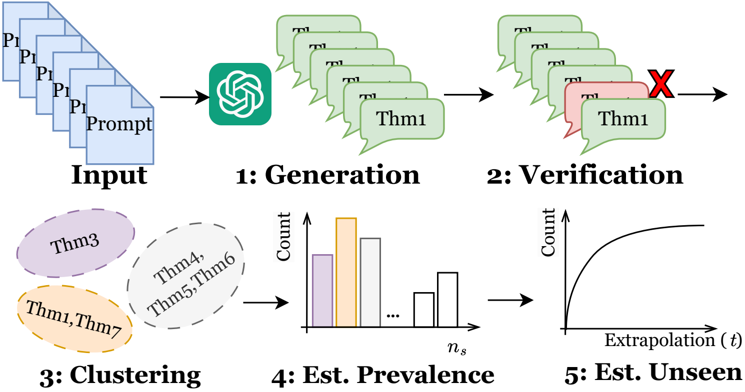


Our method [Li et al., 2025c]: Estimating the Unseen



- Five-step procedure.
- Steps 2 & 3 standardize answers.
- Verification reduces hallucination.
- Clustering reduces redundancy.
- n_0 = the amount of unseen knowledge.

Results of knowledge estimation

- Query the LLM N_{query} times with a fixed prompt, each time requesting N_{ans} instances of domain-specific knowledge.
- Use external databases for validation (e.g., Wikipedia) and cluster the responses based on their unique external identifiers (e.g., canonical URL).
- $(N_{\mathrm{query}}, N_{\mathrm{ans}}) = (30{,}000, 20)$ for theorems and $(3{,}000, 50)$ for diseases.
- $\mathrm{SKR} =$ seen knowledge / total knowledge.

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Model	**Math theorem**			**Anatomical disease**		
	N_{seen}	$\widehat{N}_{\text{tot}}$	SKR	N_{seen}	$\widehat{N}_{\text{tot}}$	SKR
① `ChatGPT-4o-chat`	702	1189	0.59	277	732	0.38
② `ChatGPT-3.5-turbo-chat`	868	1064	0.82	268	278	0.96
③ `LLaMA-V3-70B-instruct`	**1432**	**1706**	0.84	**875**	**3372**	0.26
④ `LLaMA-V3-3B-instruct`	1035	1331	0.78	780	1375	0.57
⑤ `Mistral-7B-instruct-V0.1`	753	1194	0.63	489	1723	0.28
⑥ `Qwen2.5-7B-instruct`	444	1162	0.38	426	521	0.82
⑦ `Claude-3.7-Sonnet`	120	201	0.60	115	462	**0.25**
⑧ `DeepSeek-V3`	148	241	0.61	86	334	0.26
⑨ `Gemini-1.5-flash`	100	515	**0.19**	139	143	0.97

What if we have more access to the LLM?

How LLMs combine tokens

Denote the vocabulary by $\mathcal{W} = \{1, \ldots, K\}$, a token therein by w_t, and a text by $w_{<t} := w_1 \cdots w_{t-1}$.

- **Large vocabulary**: $\mathcal{W}$ is large in practice; $K = 50,257$ for GPT-2/3.5, $= 32,000$ for LLaMa models, and $= 128,000$ for DeepSeek-R1.

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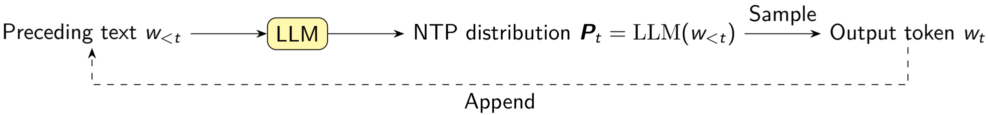
- **Large vocabulary**: $\mathcal{W}$ is large in practice; $K = 50,257$ for GPT-2/3.5, $= 32,000$ for LLaMa models, and $= 128,000$ for DeepSeek-R1.
- **Autoregresiveness**: An LLM generates each token sequentially by sampling from a probability distribution conditioned on previous tokens:

$$w_t \sim \boldsymbol{P}_t \quad \text{where} \quad \boldsymbol{P}_t = \mathrm{LLM}(w_{<t}) \quad \text{is a distribution on} \quad \mathcal{W}.$$



Example of autoregresive generation

Prefix

I saw a cat on a

$w_{1:6} = [w_1, w_2, w_3, w_4, w_5, w_6]$

LLM

$\mathbf{P}_7 = (P_{7,1}, \cdots, P_{7,K})$

Next Token, $w_7 \sim \mathbf{P}_7$

Mat	25%
Carpet	13%
Boat	5%
Plane	3%
....	...

Sampling

carpet

$\boxed{w_7}$

What if we could control the sampling of the LLM?

- By manipulating the sampling process, we can embed a statistical signal between the input (preceding text $w_{<t}$) and the output (next token w_t).
- Such dependence rarely appears in human-written text but commonly arises in LLM-generated text.

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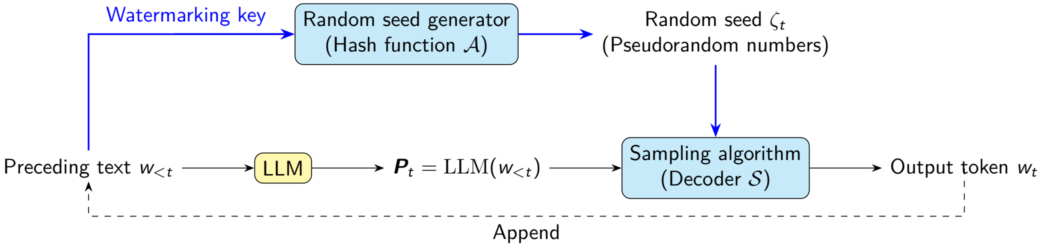
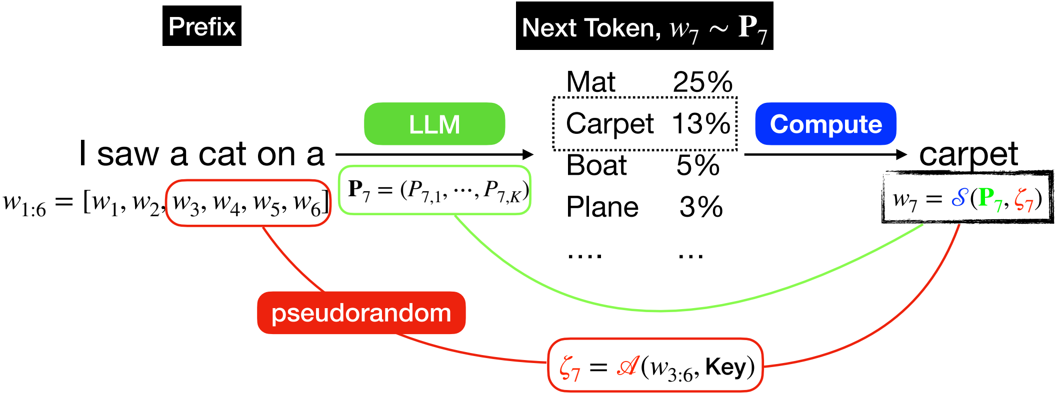
- By manipulating the sampling process, we can embed a statistical signal between the input (preceding text $w_{<t}$) and the output (next token w_t).
- Such dependence rarely appears in human-written text but commonly arises in LLM-generated text.
- This technique is known as **watermarking** [Kirchenbauer et al., 2023].
  - Enables reliable detection and attribution of AI-generated content.
  - Extends naturally to other modalities such as images and tables.
  - Many applications: AI-content labeling, academic integrity checking, biosecurity monitoring, and data provenance tracking.

Watermarked generation: Procedure



- Mathematical speaking: $\zeta_t = \mathcal{A}(w_{<t}, \mathrm{Key})$ and $w_t = \mathcal{S}(\boldsymbol{P}_t, \zeta_t)$.
- A watermark is defined by $(\mathcal{A}, \mathcal{S}, \mathrm{Key})$.
- Watermark signal is the dependence of each w_t on ζ_t.

Watermarked generation: Example



Comments on pseudorandom numbers

$\mathcal{A}(\text{public data}, \text{private info})$ computes the pseudorandom number:

- Public data $=$ prior tokens $w_{<t}$ or a segment $w_{(t-m):t}$ [Kirchenbauer et al., 2023].
- Private info $=$ secret key, denoted Key.

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Property (*Soundness of pseudorandomness*)

1. $\zeta_t = \mathcal{A}(w_{1:t-1}, \mathrm{Key})$ for $t = 1, \ldots, n$ are iid copies of a known random variable ζ
2. ζ_t is statistically independent of $w_{1:t-1}$
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  - Pseudorandom numbers are "reproducible" ***iff*** Key is known.
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  - Pseudorandom numbers are "reproducible" ***iff*** Key is known.
  - Key will be shared with the verifier through a secure protocol.
- Theory assumes true randomness; Implementation use deterministic generation.
- Similar to setting a *seed* for reproducibility in simulations.

Pseudocode for watermark embedding

Algorithm Watermarked LLM Generation

Inputs: a watermark $(\mathcal{S}, \mathcal{A}, \mathrm{Key})$ and a language model.
Load the language model $\mathrm{LLM}(\cdot)$.
Receive the user prompt s and feed it to the model to generate a continuation.
Initialize $w_{<1} = s$ and set n the maximum length.
for step $t = 1, 2, \cdots n$ **do**
    Compute the NTP distribution: $\boldsymbol{P}_t = \mathrm{LLM}(w_{<t})$.
    Compute the pseudorandom number: $\zeta_t = \mathcal{A}(w_{<t}, \mathrm{Key})$.
    Compute the next token: $w_t = \mathcal{S}(\boldsymbol{P}_t, \zeta_t)$.
    Append the history: $w_{<(t+1)} = w_{<t} w_t$. ▷ Autoregressive
return $w_{\leq n}$.

A high-level intro of watermark detection

$$H_0 : w_{\leq n} \text{ is human written} \quad \text{v.s.} \quad H_1 : w_{\leq n} \text{ is LLM-generated.}$$

- **Human-written text**: w_t is independent of ζ_t as humans don't know $\mathcal{A}$ and Key.
- **LLM-generated text**: w_t depends on ζ_t via the decoder function $\mathcal{S}$.

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Take-away

Watermarking couples each token w_t and a psedorandom ζ_t, altering their joint distribution. Pivotal statistic Y_t quantifies this evidence.

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- Practical choices uses the pivotal statistic $Y_t = Y(w_t, \zeta_t)$ [Li et al., 2025b]:
  - Under H_0, $w_t \perp \zeta_t$ such that $Y_t \sim \mu_0$.
  - Under H_1, $w_t = \mathcal{S}(\boldsymbol{P}_t, \zeta_t)$ such that $Y_t = Y(\mathcal{S}(\boldsymbol{P}_t, \zeta_t), \zeta_t) \sim \mu_{1,\boldsymbol{P}_t}$.

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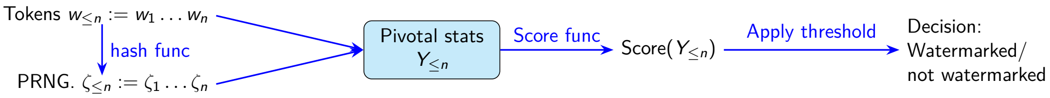

Pseudocode for watermark detection

Algorithm Watermark Detection

Inputs: a text $w_{\leq n}$, hash function $\mathcal{A}$, secret Key, and significance level α.
Simulate n iid samples from the pivotal distribution μ_0.
Set $\widehat{q}_n$ as the empirical $(1-\alpha)$-quantile of those null samples, if its theoretical counterpart is hard to compute.
Initialize $w_{<1}$ by any prefix.
for step $t = 1, 2, \cdots, n$ **do**
    Compute the pseudorandom number: $\zeta_t = \mathcal{A}(w_{<t}, \mathrm{Key})$.
    Compute the pivotal statistic: $Y_t = Y(w_t, \zeta_t)$.
Compute the test score: $T = \mathrm{Score}(Y_{\leq n})$.
Claim: LLM-generated if $T > \widehat{q}_n$ otherwise human-written.

How to optimally choose the Score function?

- For the sum-based rule $\mathrm{Score}(Y_{\le n}) = \sum_{t=1}^{n} h(Y_t)$, Li et al. [2025b] introduced an efficiency measure

$$R_{\mathcal{P}}(h) = \lim_{n\to\infty} -\frac{1}{n}\log(\text{Type II error}) \quad \text{s.t.} \quad \text{Type I error} = \alpha,$$

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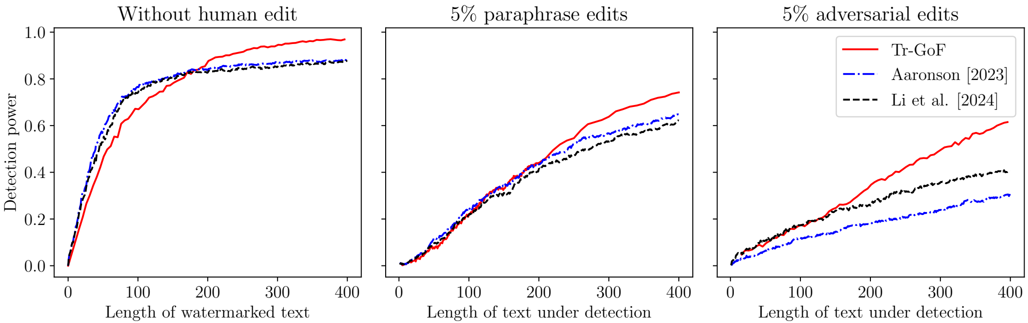
  which characterizes the exponential decay rate of the Type II error under a fixed Type I error level.
- Maximizing $R_{\mathcal{P}}(h)$ over h yields the optimal detection rule when all NTP distributions are contained in a given class $\mathcal{P}$.
- Li et al. [2025a] proposed a truncated goodness-of-fit (GoF) test for corruption scenarios and proved its optimality in certain regimes.
- He et al. [2025] demonstrated that general GoF tests enhance both detection power and robustness to corruption.
- Cai et al. [2025] derived the optimal score function in settings where the pseudorandom variables are not i.i.d.

Performance of different detectors

- On C4 news-like dataset [Raffel et al., 2020] and OPT-1.3B model [Zhang et al., 2022] (temperature 0.3).



A self-contained watermark python demo

- **Download**:
  https://github.com/lx10077/WatermarkFramework/blob/main/watermark_demo.py
- **How to use**:
  `python watermark_demo.py -temp 1 -alpha 0.01 -model facebook/opt-1.3b`

```
tokenizer = AutoTokenizer.from_pretrained(args.model) # Load tokenizer which convers text to a sequence of
# Ensure the tokenizer has a pad token
if tokenizer.pad_token is None:
    tokenizer.pad_token = tokenizer.eos_token
model = AutoModelForCausalLM.from_pretrained(
    args.model,
    device_map="auto",              # Automatically place model layers on available GPU(s)
    torch_dtype=torch.float16       # (Optional) Set tensor data type to float16 for faster computation
)
device = torch.device("cuda" if torch.cuda.is_available() else "cpu") # Use GPU if possible
print(f"Using device: {device}")
model = model.to(device) # Move the model to GPU, otherwise it is default on CPU
model.eval()

# Load the first 200 samples from the AG News dataset.
# You could also test your own questions or queries. The model will continue to write after your given tex
# To that end, simply change the following 'raw_texts' with a list of your questions.
dataset = load_dataset("ag_news", split="train[:200]")
```

Concluding remarks

- Even with only API access, we can still conduct meaningful research. For example, estimate unseen knowledge.
- Watermarking enhances content traceability and integrity by coupling each toke with tractable pseudorandom numbers.
- Many interesting statistical challenges emerge in practical watermarking applications:

Whether watermarked → How many watermarked → Which watermarked

- Have a try to watermark!

  https://github.com/lx10077/WatermarkFramework/blob/main/watermark_demo.py

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