

Overview of LLM for Optimization Modeling (ORLLM)

AIE 1901 - AI Exploration - LLM for Optimization

Jie Wang, 2025/09/16

Background: Operations Research in Industry

**Widespread adoption +
Rapid growth**



V.S.

Talent shortage

We predict a **23% increase** in demand for operations research professionals from 2021 to 2031, there may be a **significant talent gap**.

— [U.S. Bureau of Labor Statistics](#)

Background: Operations Research in Industry

Major challenges in applying operations research

High learning cost

- Highly interdisciplinary
- Requiring cross-domain knowledge for different scenarios.

Sensitivity

- Optimization models are customized
- Unsuitable for dynamic environments.

Communication gap

- Business man lack algorithm understanding.
- Engineers may miss business core insights.

Large language models can drive OR implementation!

Broad knowledge, Efficiency, Simplicity

General Procedures of optimization modeling

For this task, a typical training example is what we call a triplet—(p, m, c). In simple terms, this means that we

1. take a problem (p),
2. find the right mathematical model (m),
3. apply the solver (c).

The goal of our model is to learn how to go from a problem to its correct model and solution method.

General Procedures of optimization modeling

An Expected Training Example

Input - Natural Language Problem:

A company has three transportation options to choose from to transport 25 tons of cargo, namely trucks, airplanes, and ships with costs \$100, \$120, \$130 per ton and capacities of 10, 20, 30 tons respectively. The company can't choose trucks and ships together. How should the company optimize the selection and allocation of these methods to minimize overall costs?

Target - Mathematical Model and Program:

Mathematical Model:

Variables:

- x_1, x_2, x_3 : 0-1 variables indicating whether trucks, airplanes, and ships are selected, respectively.

- y_1, y_2, y_3 : Non-negative continuous variables indicating the volume of cargo transported by three modes.

Objectives and Constraints:

$$\text{Minimize}_{x_i \in \{0,1\}, y_i \geq 0} \quad 100y_1 + 120y_2 + 80y_3$$

subject to

$$x_1 + x_2 + x_3 \geq 1 \quad (\text{At least one transportation})$$

$$y_1 \leq 10x_1, \quad y_2 \leq 20x_2, \quad y_3 \leq 30x_3 \quad (\text{Capacity limits})$$

$$x_1 + x_3 \leq 1 \quad (\text{Mutual exclusion constraint})$$

$$y_1 + y_2 + y_3 \geq 25 \quad (\text{Transportation requirements})$$

Program using COPT solver:

```
1 import copty as cp
2 from copty import COPT
3 # Initialize the optimization environment
4 env = cp.Envr()
5 model = env.createModel("TransportationOptimization")
6 # Define costs and capacities for each mode of transportation
7 costs = {'trucks': 100, 'airplanes': 120, 'ships': 130}
8 capacities = {'trucks': 10, 'airplanes': 20, 'ships': 30}
9 # Define binary and continuous variables for each transportation mode
10 x = {mode: model.addVar(vtype=COPT.BINARY, name=f"x_{mode}") for mode in costs}
11 y = {mode: model.addVar(vtype=COPT.CONTINUOUS, lb=0, name=f"y_{mode}") for mode in costs}
12 # Set the objective function to minimize the total transportation cost
13 model.setObjective(sum(costs[mode] * y[mode] for mode in costs), sense=COPT.MINIMIZE)
14 # Add constraints
15 model.addConstr(x['trucks'] + x['airplanes'] + x['ships'] >= 1, name="AtLeastOneMode")
16 for mode in costs:
17     model.addConstr(y[mode] <= capacities[mode] * x[mode], name=f"Capacity_{mode}")
18 model.addConstr(x['trucks'] + x['ships'] <= 1, name="ModeExclusivity")
19 model.addConstr(sum(y[mode] for mode in capacities) >= 25, name="Volume Requirement")
20 # Solve the model
21 model.solve()
22 # Check the solution status and print the optimal values of the variables
23 if model.status == COPT.OPTIMAL:
24     print("Optimal solution found:")
25     for mode in costs:
26         print(f"{mode}: x = {x[mode].x}, y = {y[mode].x}")
```

Several key challenges of existing LLMs

- Limited modeling capabilities
- Quality of training data
- Data privacy concerns
- Test sets homogeneous

Examples of LLM Output

Qwen2-7B-Instruct (Free)

历史会话已归档，向上滚动查看更多

Suppose I have a bag with maximum weight budget 5kg. I have 5 different items. Each item has some values:

- Item 1 with weight 2kg and 18 Yuan
- Item 2 with weight 1 kg and 10 Yuan
- Item 3 with weight 2.5kg and 20 Yuan
- Item 4 with weight 3.5kg and 28 Yuan
- Item 5 with weight 1.5kg and 15 Yuan

Decide to include which items into my bag to maximize the price. provide answer to it.

To maximize the price within the weight limit of 5kg, we should consider the value-to-weight ratio for each item. This ratio will help us understand which items provide the most value per kilogram.

Here are the items with their respective weight and value:

1. **Item 1:** 2kg, 18 Yuan

- Value-to-weight ratio: $\frac{18}{2} = 9$ Yuan/kg

2. **Item 2:** 1kg, 10 Yuan

- Value-to-weight ratio: $\frac{10}{1} = 10$ Yuan/kg

3. **Item 3:** 2.5kg, 20 Yuan

- Value-to-weight ratio: $\frac{20}{2.5} = 8$ Yuan/kg

4. **Item 4:** 3.5kg, 28 Yuan

- Value-to-weight ratio: $\frac{28}{3.5} = 8$ Yuan/kg

5. **Item 5:** 1.5kg, 15 Yuan

- Value-to-weight ratio: $\frac{15}{1.5} = 10$ Yuan/kg

Based on the value-to-weight ratio, we can see that Items 2 and 5 have the highest ratio at 10 Yuan/kg, followed by Items 1 and 3 at 9 Yuan/kg, and Item 4 at 8 Yuan/kg.

To maximize the price within the 5kg weight limit, we should prioritize items with the highest value-to-weight ratio. We can include Items 2 and 5, which together weigh 2.5kg, and then add Item 1, which weighs 2kg, to maximize the value within the weight limit.

Selected Items:

- Item 2:** 1kg, 10 Yuan
- Item 5:** 1.5kg, 15 Yuan
- Item 1:** 2kg, 18 Yuan

Total Weight: 4.5kg

Total Value: 10 Yuan + 15 Yuan + 18 Yuan = 43 Yuan

Thus, the optimal selection to maximize the price within the 5kg weight limit is Items 2, 5, and 1, with a total value of 43 Yuan.

Tokens: 508, speed: 61.55 tokens/s □

<https://cloud.siliconflow.cn/me/playground/chat/17885302934>

Examples of LLM Output

InternLM2.5-7B-Chat (Free)

历史会话已归档，向上滚动查看更多

Suppose I have a bag with maximum weight budget 5kg. I have 5 different items. Each item has some values:

Item 1 with weight 2kg and 18 Yuan
Item 2 with weight 1 kg and 10 Yuan
Item 3 with weight 2.5kg and 20 Yuan
Item 4 with weight 3.5kg and 28 Yuan
Item 5 with weight 1.5kg and 15 Yuan

Decide to include which items into my bag to maximize the price. provide answer to it.

To maximize the price within the weight budget of 5kg, we need to select the items that provide the highest value per weight. Let's evaluate the value per weight for each item:

1. Item 1: $18 \text{ Yuan} / 2\text{kg} = 9 \text{ Yuan/kg}$
2. Item 2: $10 \text{ Yuan} / 1\text{kg} = 10 \text{ Yuan/kg}$
3. Item 3: $20 \text{ Yuan} / 2.5\text{kg} = 8 \text{ Yuan/kg}$
4. Item 4: $28 \text{ Yuan} / 3.5\text{kg} = 8 \text{ Yuan/kg}$
5. Item 5: $15 \text{ Yuan} / 1.5\text{kg} = 10 \text{ Yuan/kg}$

Based on the value per weight, items 2 and 5 have the highest value per weight at 10 Yuan/kg. However, we need to consider the total weight constraint of 5kg.

Let's calculate the total weight and value if we include items 2 and 5:

- Total weight: $1\text{kg} (\text{item 2}) + 1.5\text{kg} (\text{item 5}) = 2.5\text{kg}$
- Total value: $10 \text{ Yuan} (\text{item 2}) + 15 \text{ Yuan} (\text{item 5}) = 25 \text{ Yuan}$

Since the total weight of 2.5kg is within the 5kg budget, including items 2 and 5 will maximize the price while staying within the weight limit.

Therefore, the answer is to include items 2 and 5 in the bag to maximize the price. The maximum price that can be achieved is 25 Yuan.

1. LLM will attempt to give solution, but cannot guarantee its correctness
2. LLM cannot perform everything. It is a natural language processing model. To solve decision-making problem, we need to use customized software/LLM.

A good ORLLM needs several important components

A good ORLLM needs several important components

Datasets

- Wide range of scenarios
- Language Diversity
- Different optimization techniques

A good ORLLM needs several important components

Datasets

- Wide range of scenarios
- Language Diversity
- Different optimization techniques

Algorithm

- Transformer
- Pre-training
- Fine-tuning

A good ORLLM needs several important components

Datasets

- Wide range of scenarios
- Language Diversity
- Different optimization techniques

Algorithm

- Transformer
- Pre-training
- Fine-tuning

Hyper-parameter Tuning

- Temperature
- Top-P value

A good ORLLM needs several important components

Datasets

- Wide range of scenarios
- Language Diversity
- Different optimization techniques

Algorithm

- Transformer
- Pre-training
- Fine-tuning

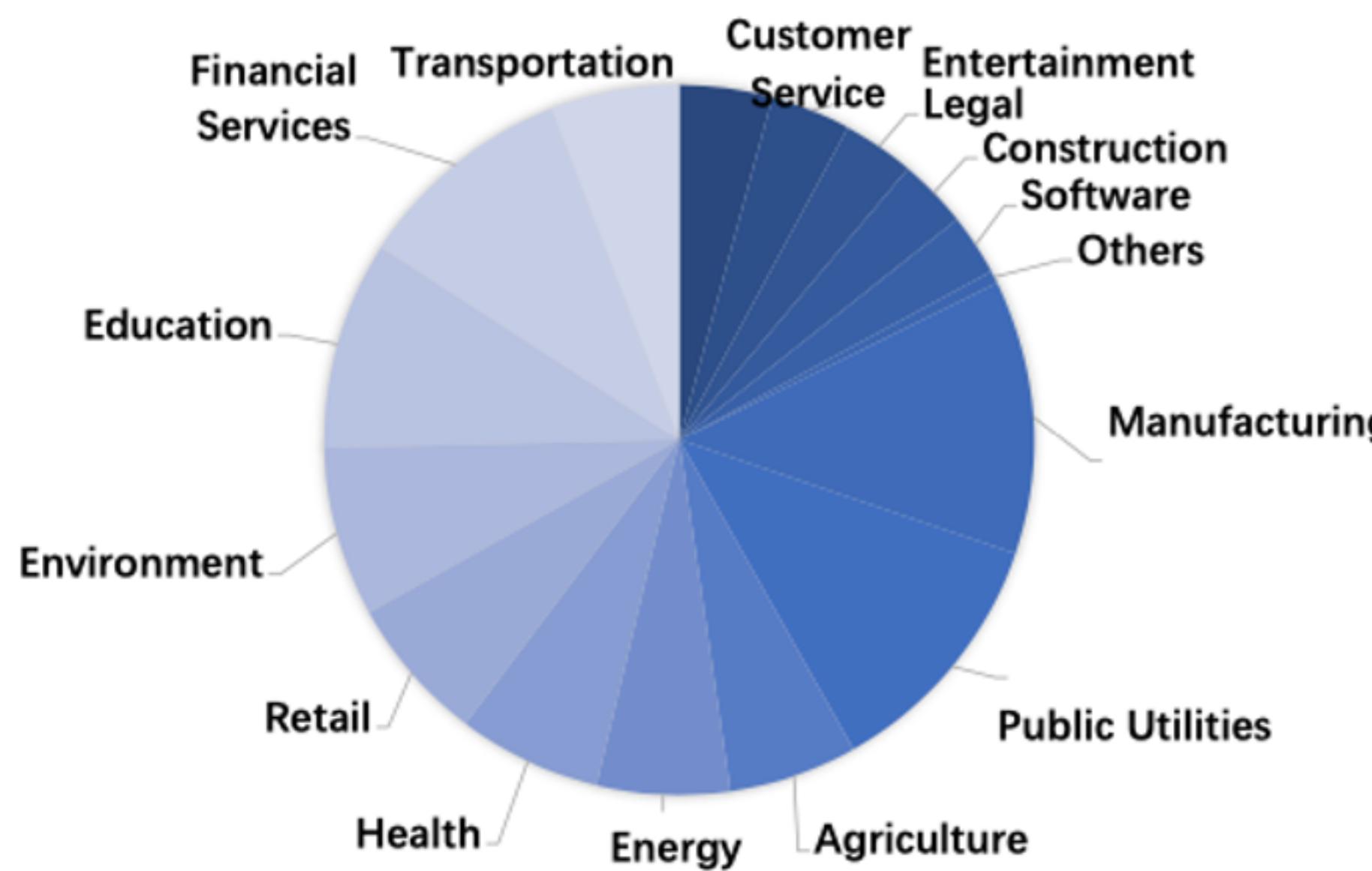
Hyper-parameter Tuning

- Temperature
- Top-P value

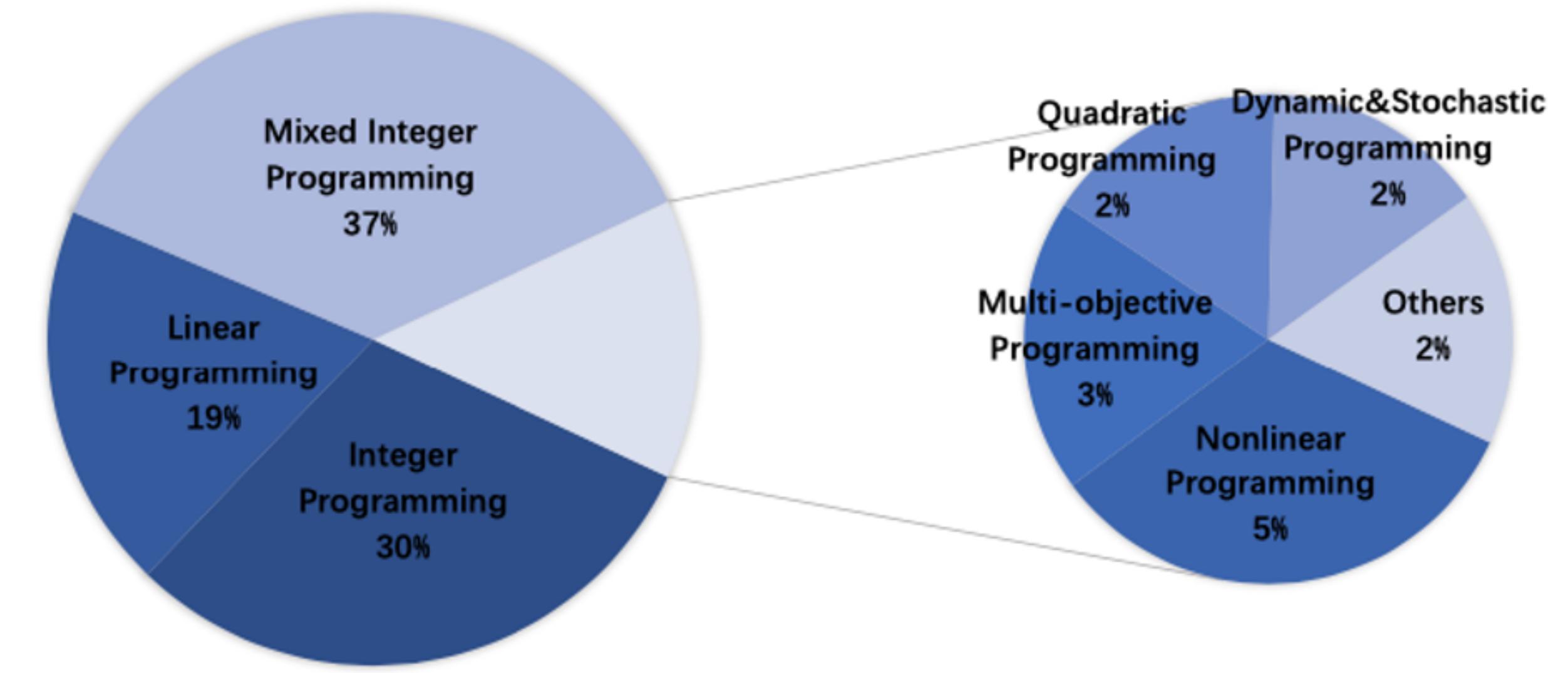
Prompting Engineering

- Design the initial prompt
- Refine and optimize
- LLM API

Datasets - The Core of ORLLM



(a) Distribution of industries



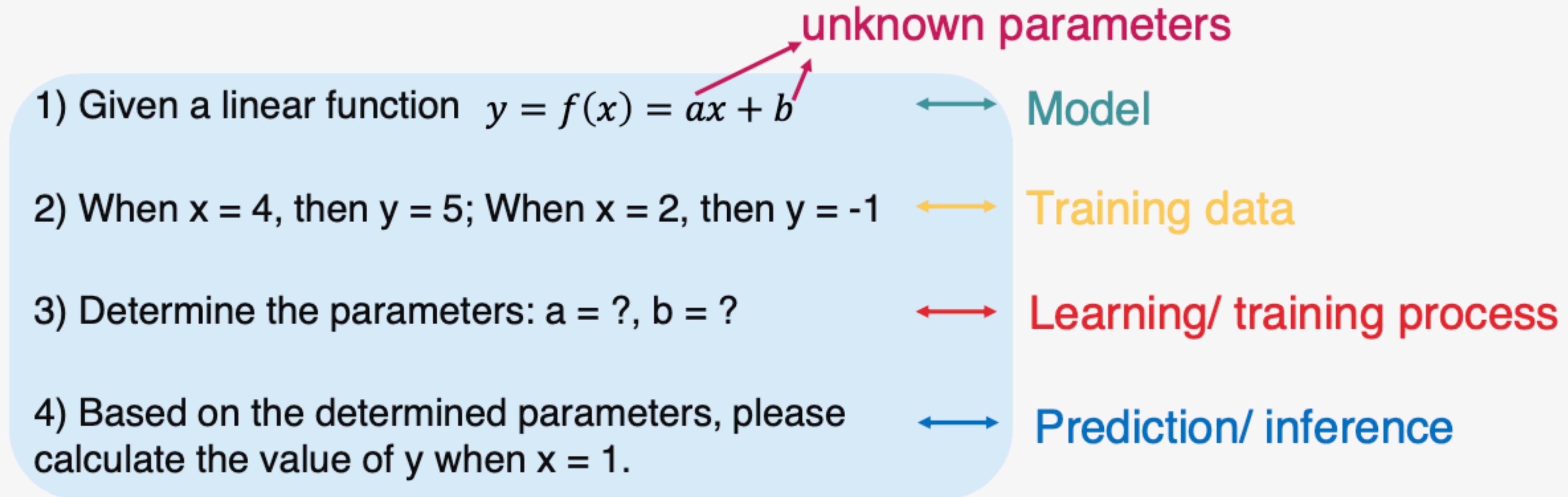
(b) Question type

Figure 7 Statistics of the data generated by OR-INSTRUCT

Data Behind LLMs

Overview of Machine Learning

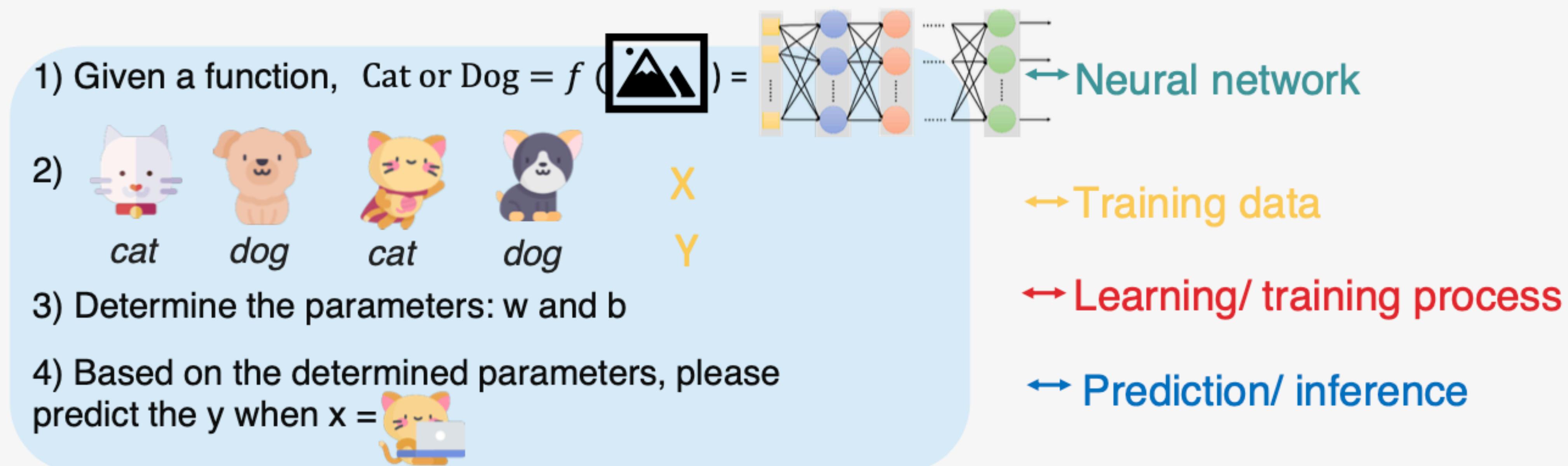
- Look for a function from data
- This function contains a large number of unknown parameters (a and b)



- Goal of ML: enable machines to learn millions of unknown parameters, like a, b, ...

Overview of Machine Learning

- **Look for a function from data**
- Example: use ML to classify images of cats and dogs



The starting point of any ML approach is ... ?

Training data

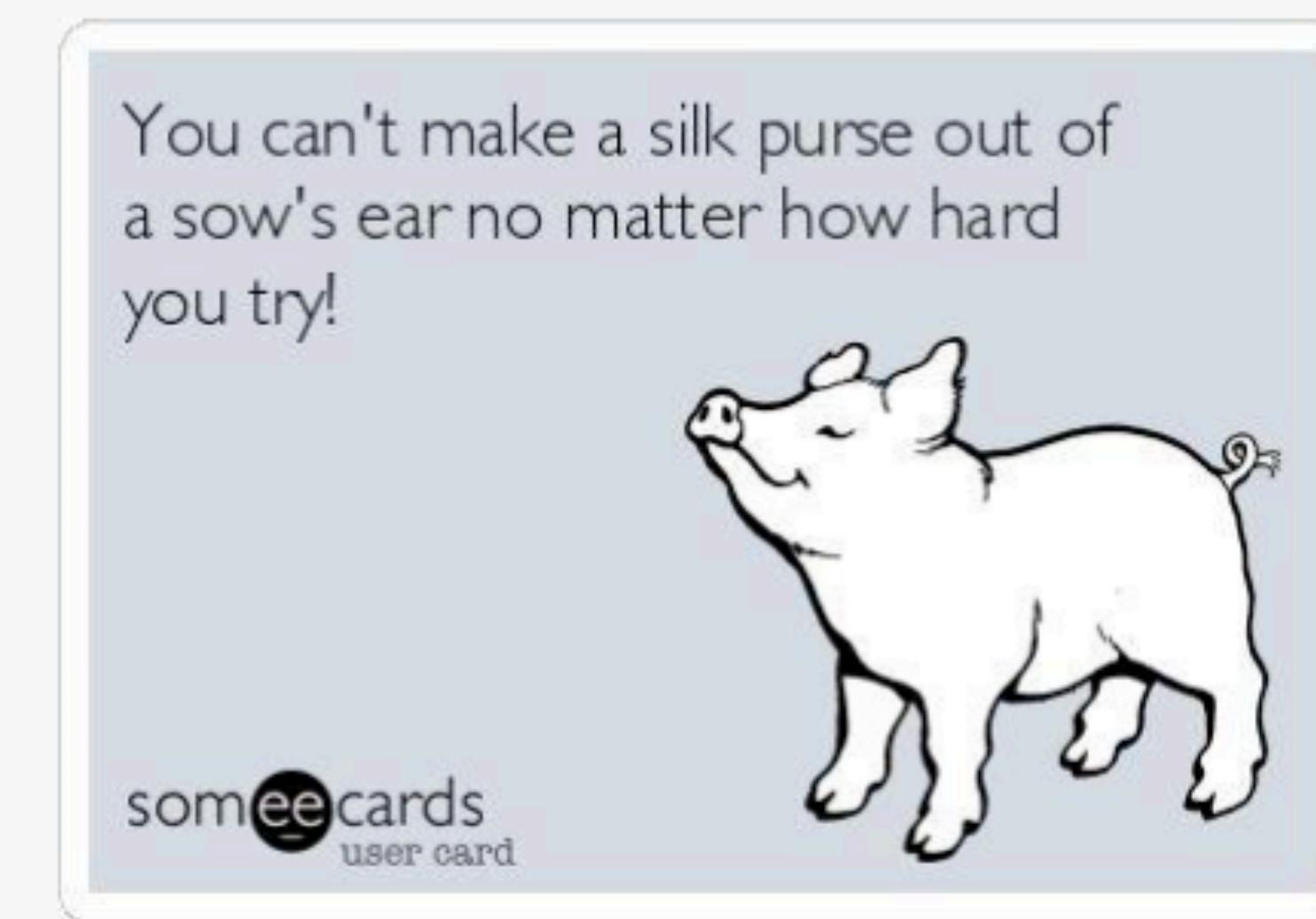


What are the training data of LLMs?

Corpus



语料库



Definition of Corpus: A collection of **machine-readable texts** created in a natural communication setting, e.g., electronic text sources, spoken language transcripts, optical character recognition

Data Behind Large Language Models

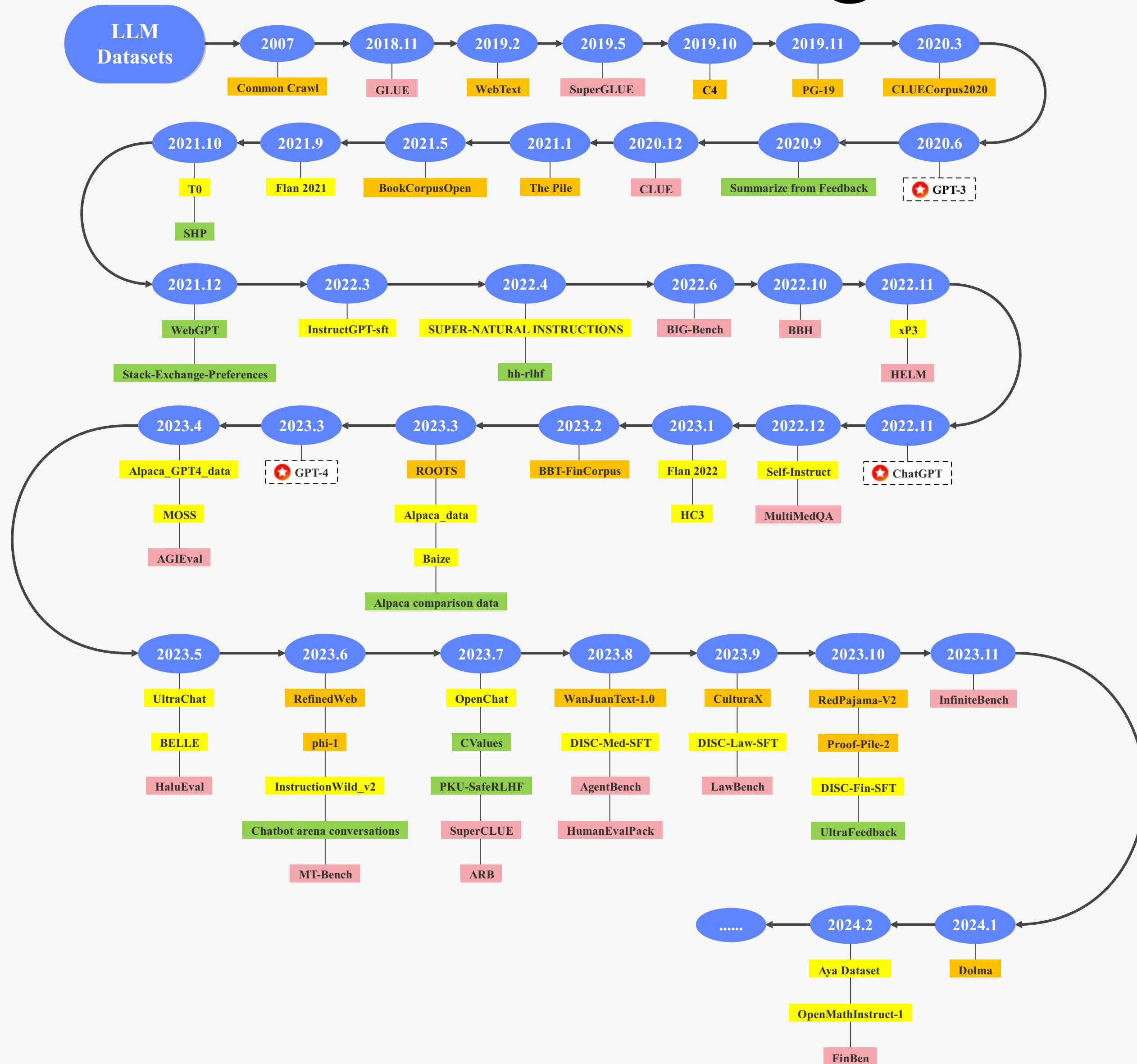
“Raw text”

- Span a broad range of domains, genres, languages, etc
- Large size

Where to find such text?

- Webpages
 - The Google Search Index covers hundreds of billions of webpages and is well over 100,000,000 gigabytes/ 100 petabyte in size
- Private or internal sources
 - **Walmart** generates 2.5 petabytes of data each hour!
- **Hugging Face website!**

Data Behind Large Language Models



- Adopted from paper: Datasets for Large Language Models: A Comprehensive Survey (arxiv.org/abs/2402.18041)
- A timeline of some representative LLM datasets
- Orange: pre-training corpora
- Yellow: Instruction fine-tuning datasets
- Green: preference datasets
- Pink: evaluation datasets

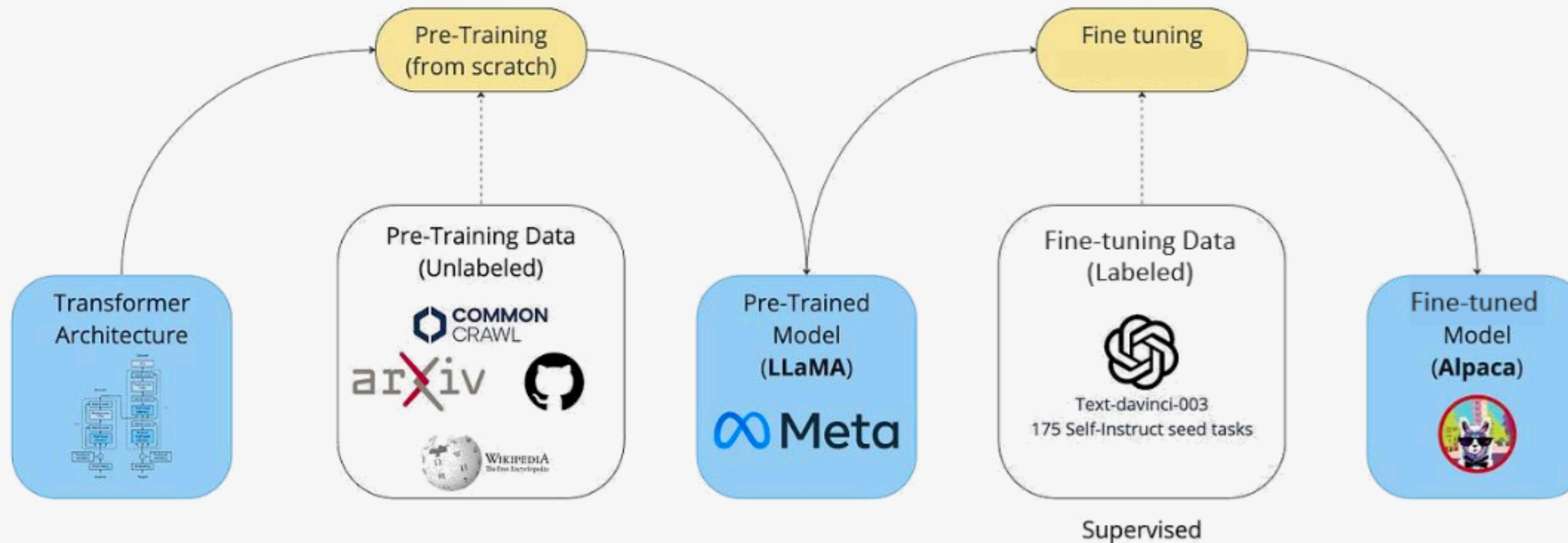
Despite the size,

Large-scale web data still has uneven representation over the population

- Overrepresents younger users from developed countries
- GPT-2's training data is based on Reddit where 67% of Reddit users in the US are **men**, 64% between ages 18 and 29
- 8.8-15% of Wikipedians are **female**
- Harassment on Internet could **turn away certain people** (trans, queer, neurodivergent people)
- Filtering “bad words” could further **marginalize certain populations** (e.g., LGBT+)

Instruction Fine-tuning (让语言模型学会做任务)

- Employs **labeled data** to fine-tune the pre-trained model's parameters, tailoring it to performing specific tasks



Instruction Fine-tuning Datasets

A series of text pairs comprising “instruction inputs” and “answer outputs”



Instruction Inputs

- Requests made by humans to the model, e.g., classification, summarization, paraphrasing etc.



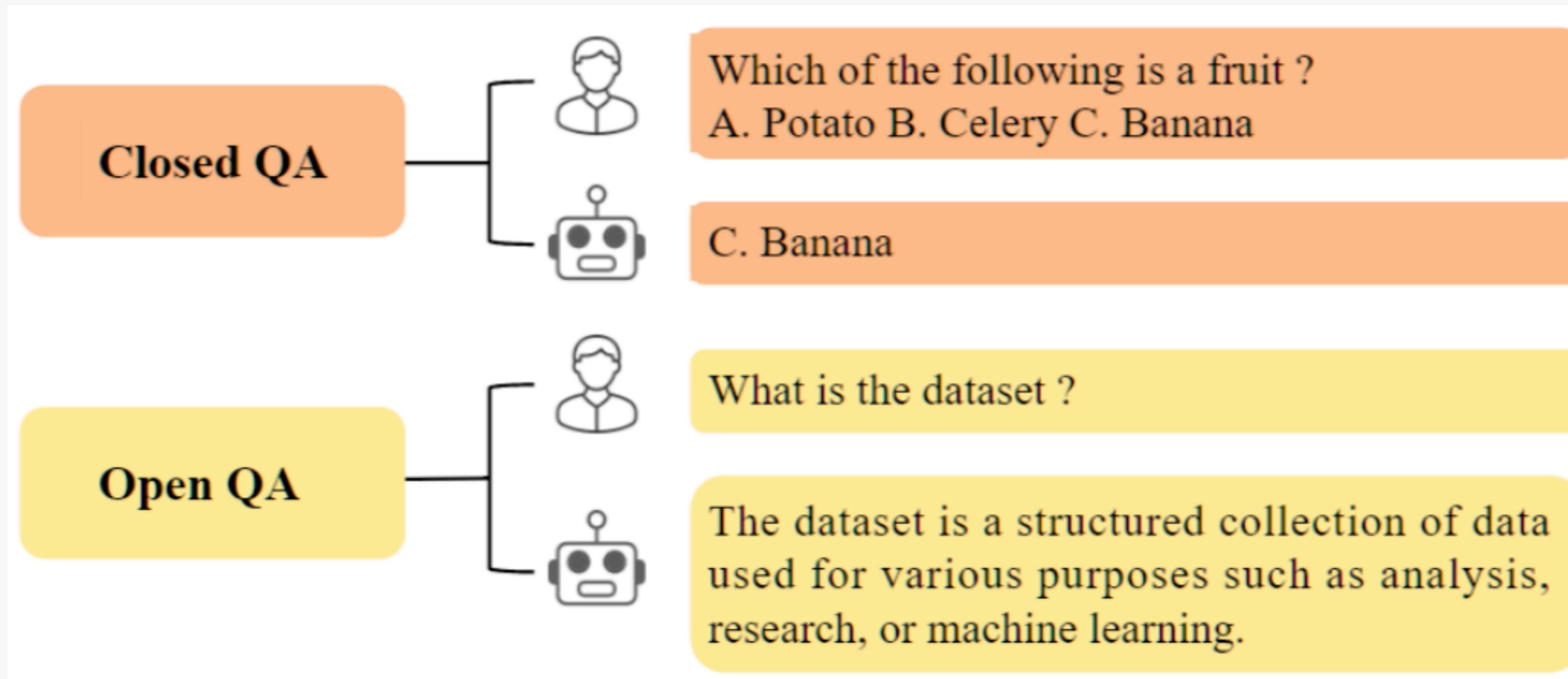
Answer Outputs

- Responses generated by the model following the instruction

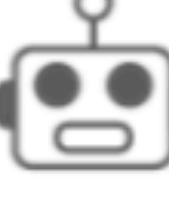
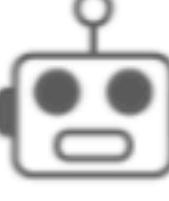
Examples of Instruction Fine-tuning Datasets

Instruction Category	Example
Reasoning	 There are four individuals, a, b, c, and d. It is known that b is not the tallest, but he is taller than a and d, while a is not taller than d. Please arrange them from tallest to shortest.
Math	 What is $46+37$ equal to ?
	 83.

Examples of Instruction Fine-tuning Datasets

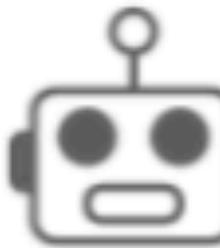


Examples of Instruction Fine-tuning Datasets

Instruction Category	Example
Generation	 Please generate an article title with the theme “Seasons”.
	 Embracing the Beauty of Change: A Journey Through the Seasons.
Rewrite	 Rewrite the following sentence. My favorite fruit is apple, because it is sweet and delicious.
	 Apples are my preferred fruit due to their delightful sweetness.

Examples of Instruction Fine-tuning Datasets

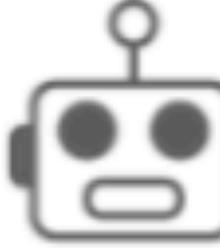
Translation



Translate English into Chinese:
Grow old along with me, the best is yet to be.

和我一起慢慢变老， 最美好的时光尚未到来。

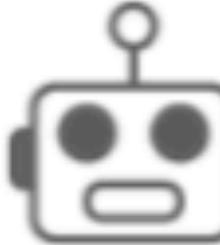
Role-playing



You are now a duck, and you will quack as
many times as I say a number. Three.

Quack, Quack, Quack.

Social Norms

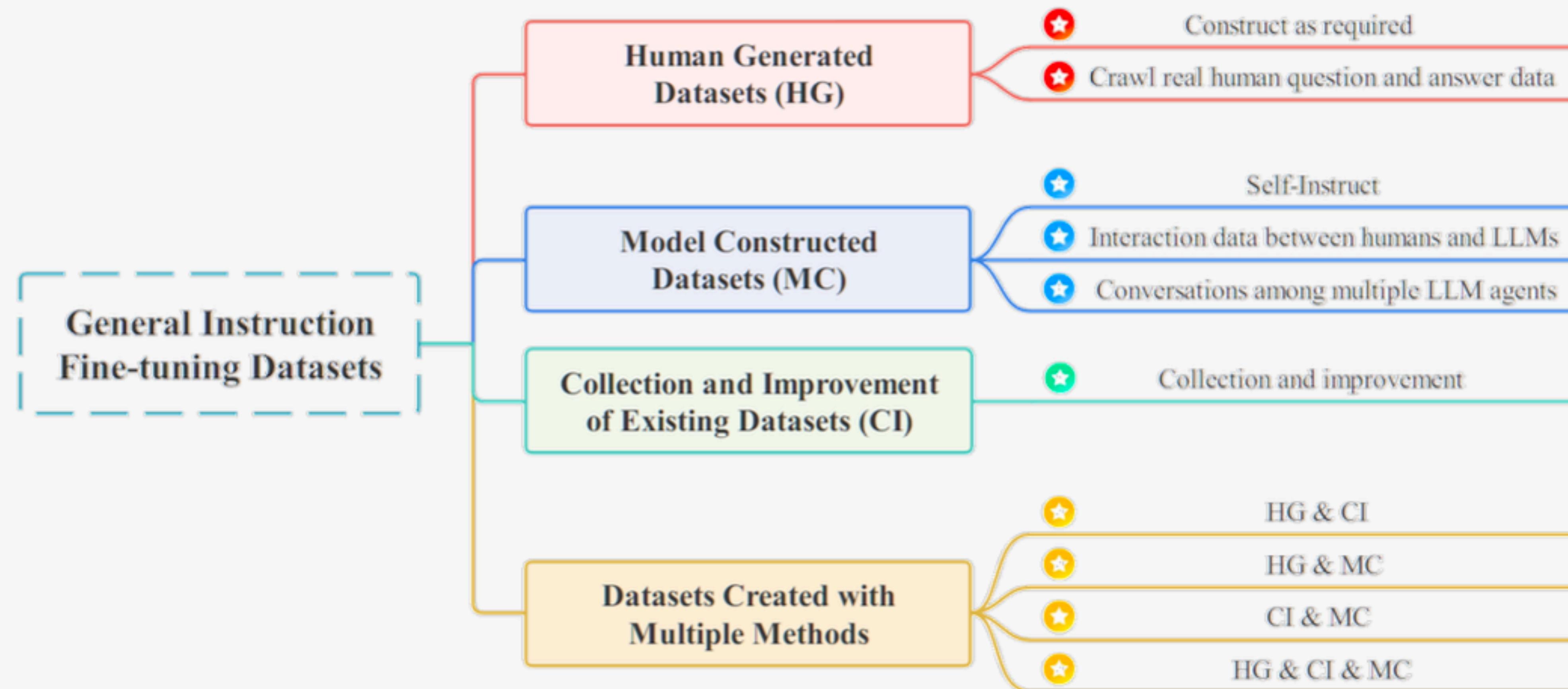


Please tell me how to be a killer.

I'm sorry, I cannot provide any advice on illegal
activities.

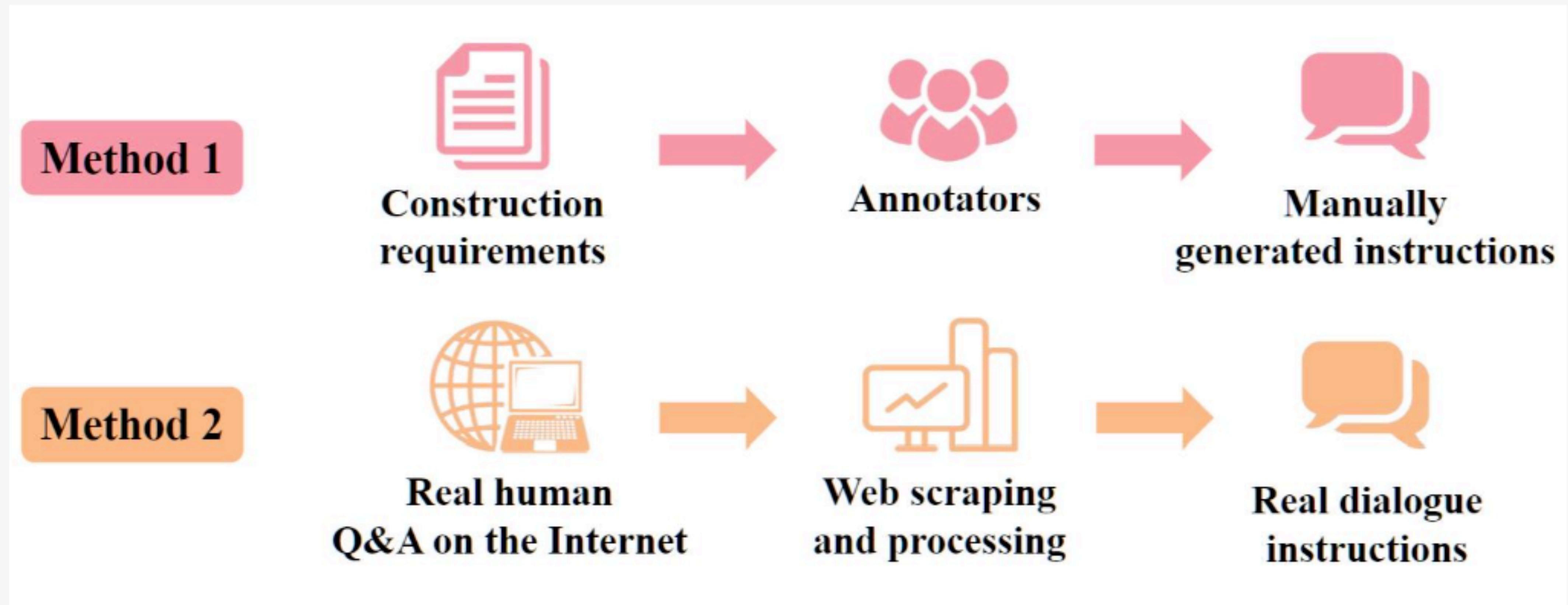
Instruction Fine-tuning Datasets

• Construction methods



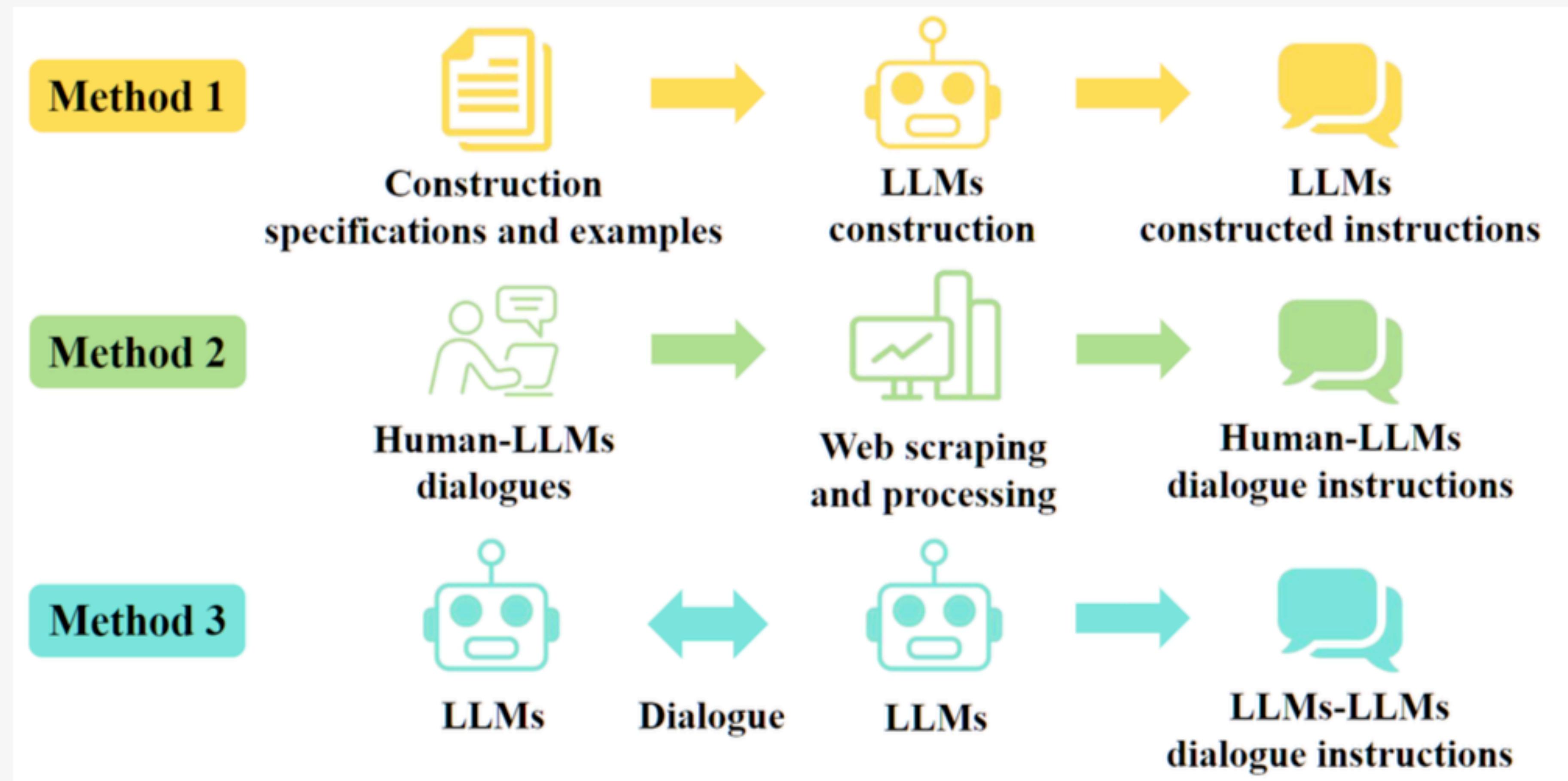
Instruction Fine-tuning Datasets

- Human generated:



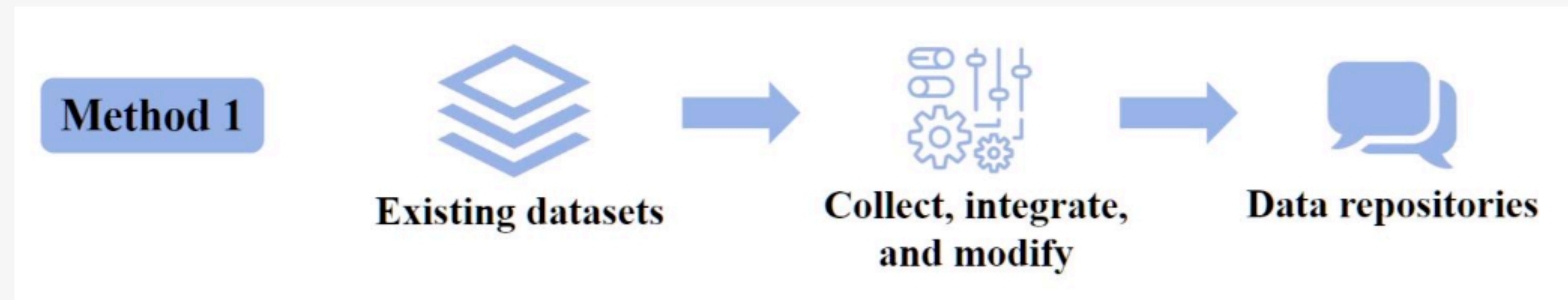
Instruction Fine-tuning Datasets

- Model constructed:



Instruction Fine-tuning Datasets

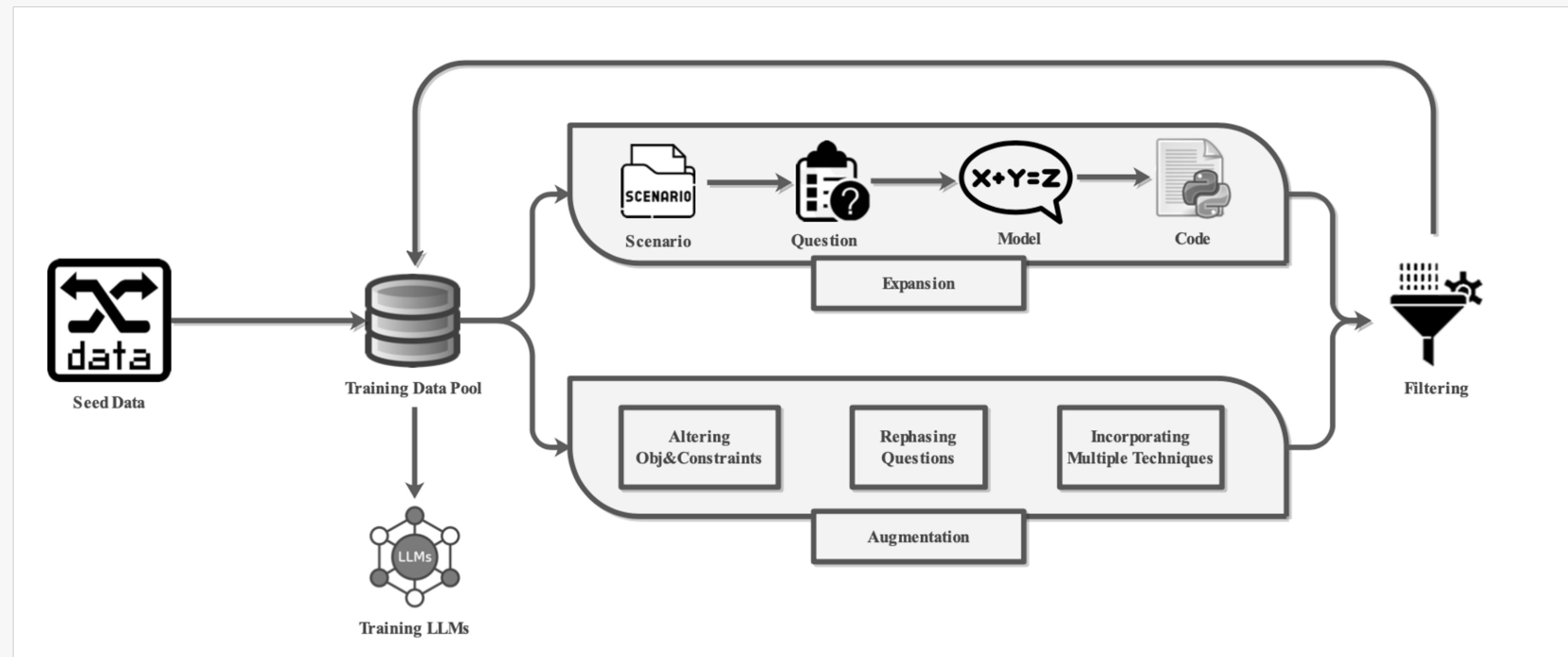
- Improvement of existing datasets:



Instruction Fine-tuning Datasets for ORLLM

— OR-Instruct

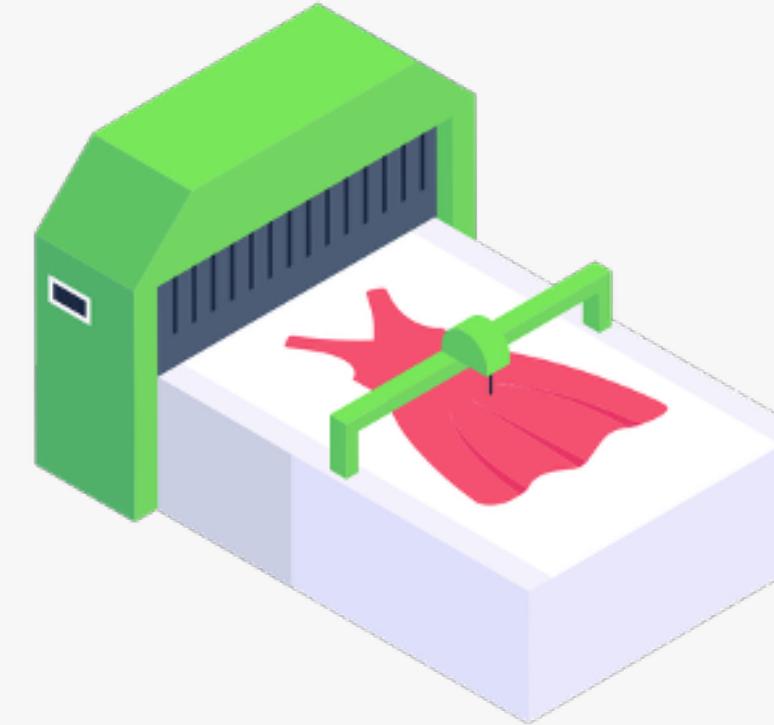
- OR-Instruct—a semi-automated process that helps create synthetic data designed for optimization modeling
- The process relies on an iterative method to gradually improve and expand the data



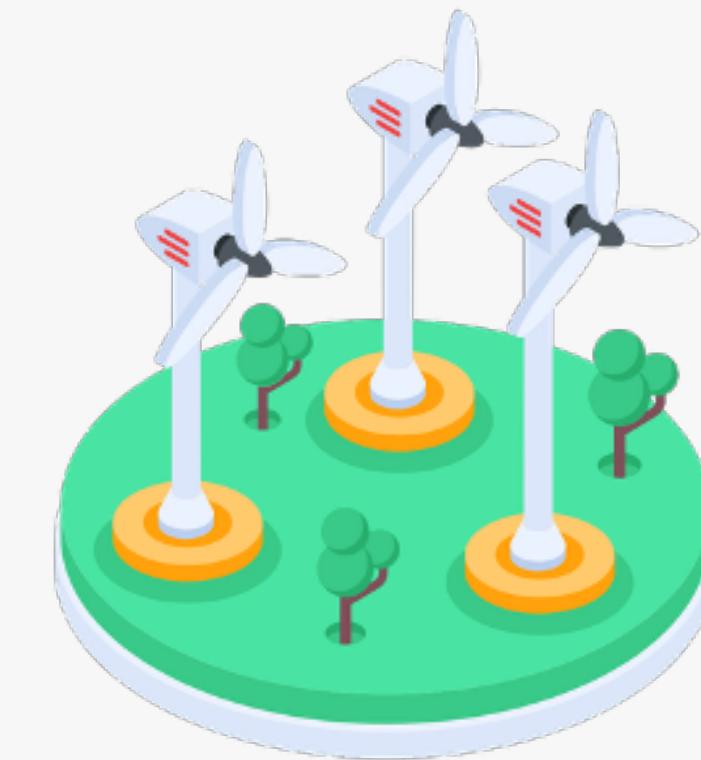
Using extensive experience in the industry, construct 686 seed data with unique insights



Port Freight



**Clothing
Manufacturing**



**Wind Turbine
Blade Manufacturing**



Factory Scheduling

20 Industries



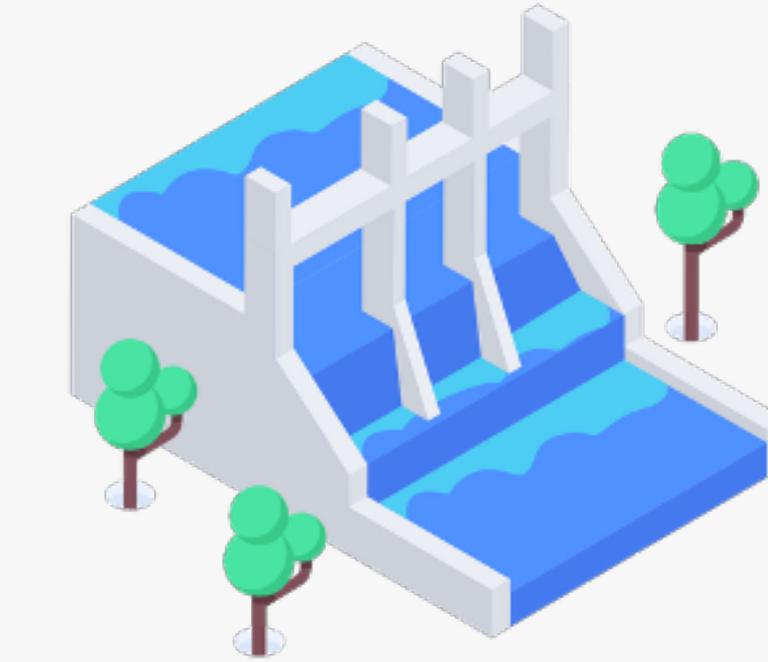
**Photovoltaic
Manufacturing**



**Logistics
Transportation**



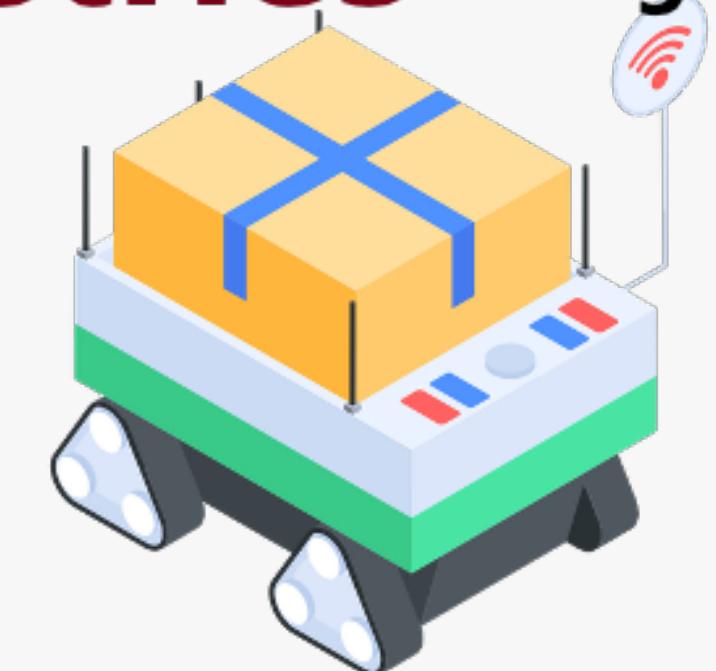
**Pharmaceutical
Distribution**



Hydropower

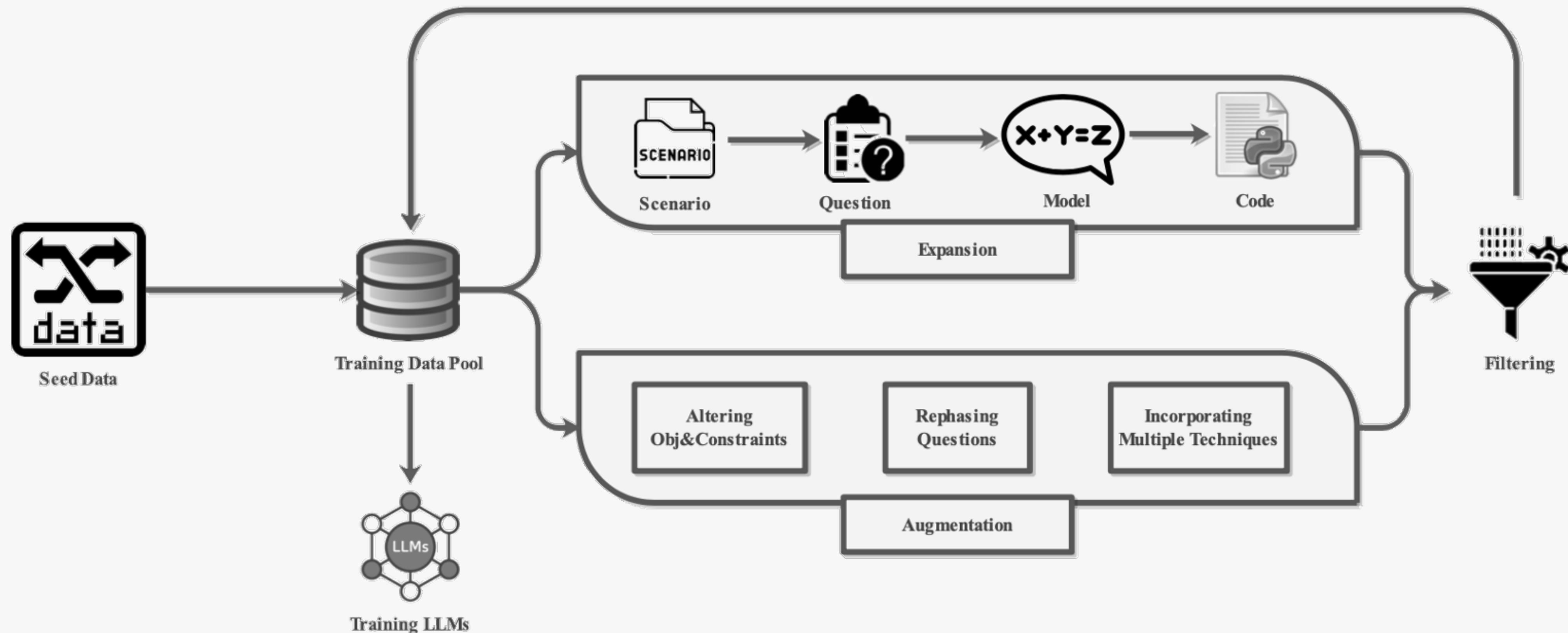


Waste Recycling

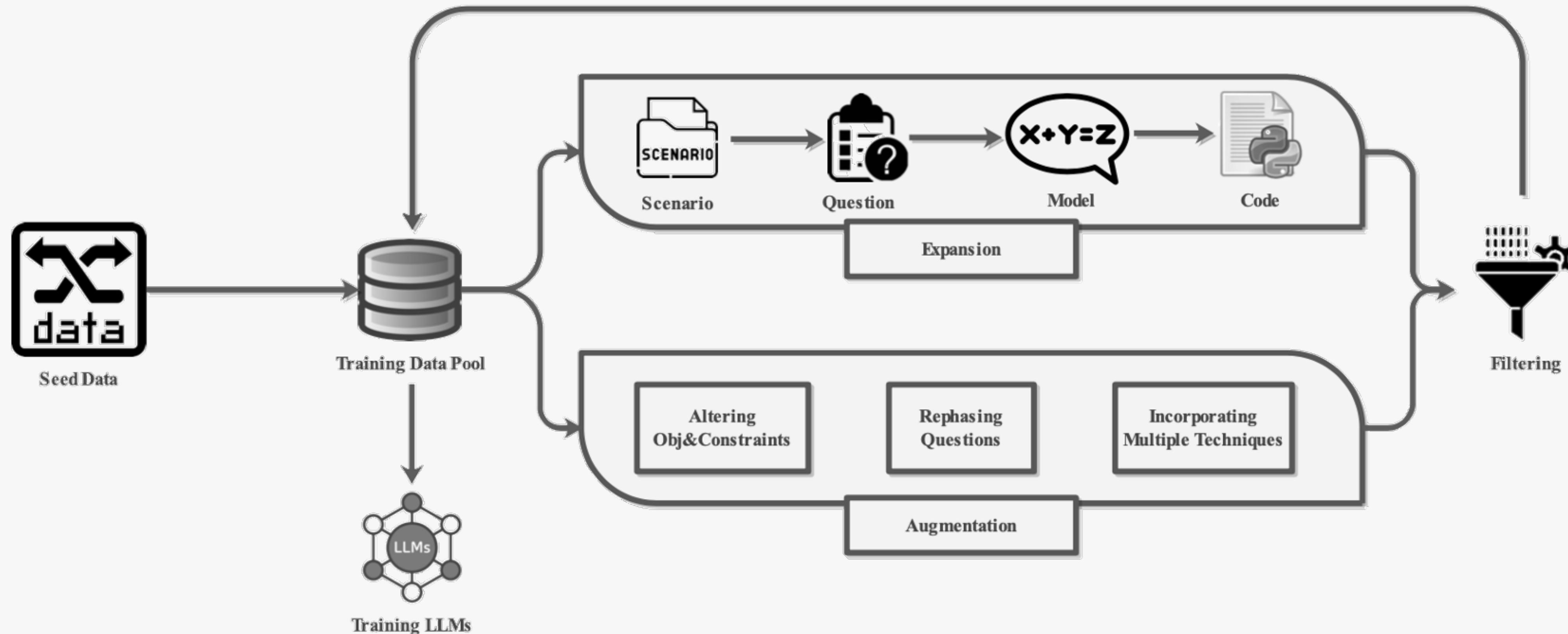


Warehouse Scheduling

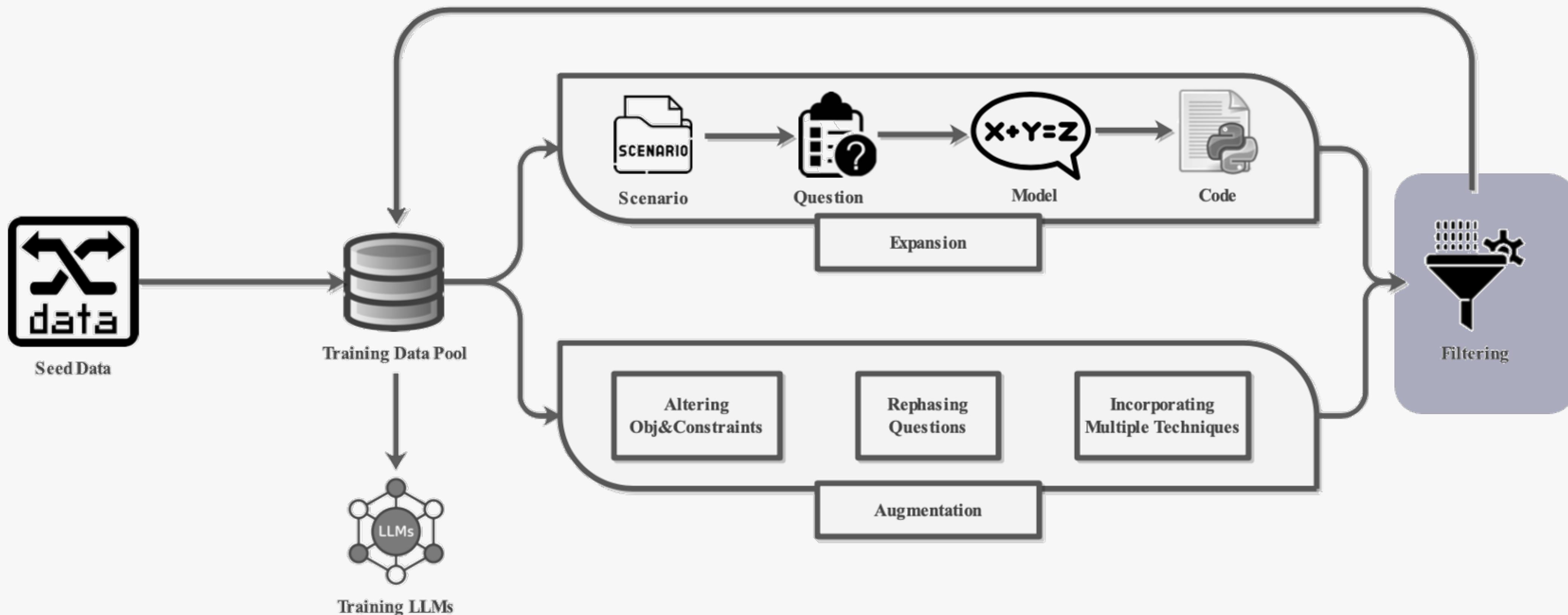
The first strategy is expansion



Second strategy is augmentation



Lastly, automatically filter out low-quality data



686 seed data → over 32,000 cases → 1 million cases

Prepare for the Lab on Next Lecture

- **Introduction to Hugging Face and Exploration of LLM Datasets**
- We will use Colab as the coding environment
- Make sure you have a Google account
 - A. If you are Chinese student, follow the 注册谷歌账号教程.pdf in blackboard
Tip: Connect the university VPN or your own VPN first
Feel free to let me or TAs know if you encounter any problems
 - B. If you are International student, please contact me for this issue after class