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scGPT: towards building a foundation model for single-cell multi-omics using generative AI

Authors: Haotian Cui*, Chloe Wang*, Hassaan Maan, Kuan Pang, Fengning Luo, Bo Wang

Present by: Haotian Cui

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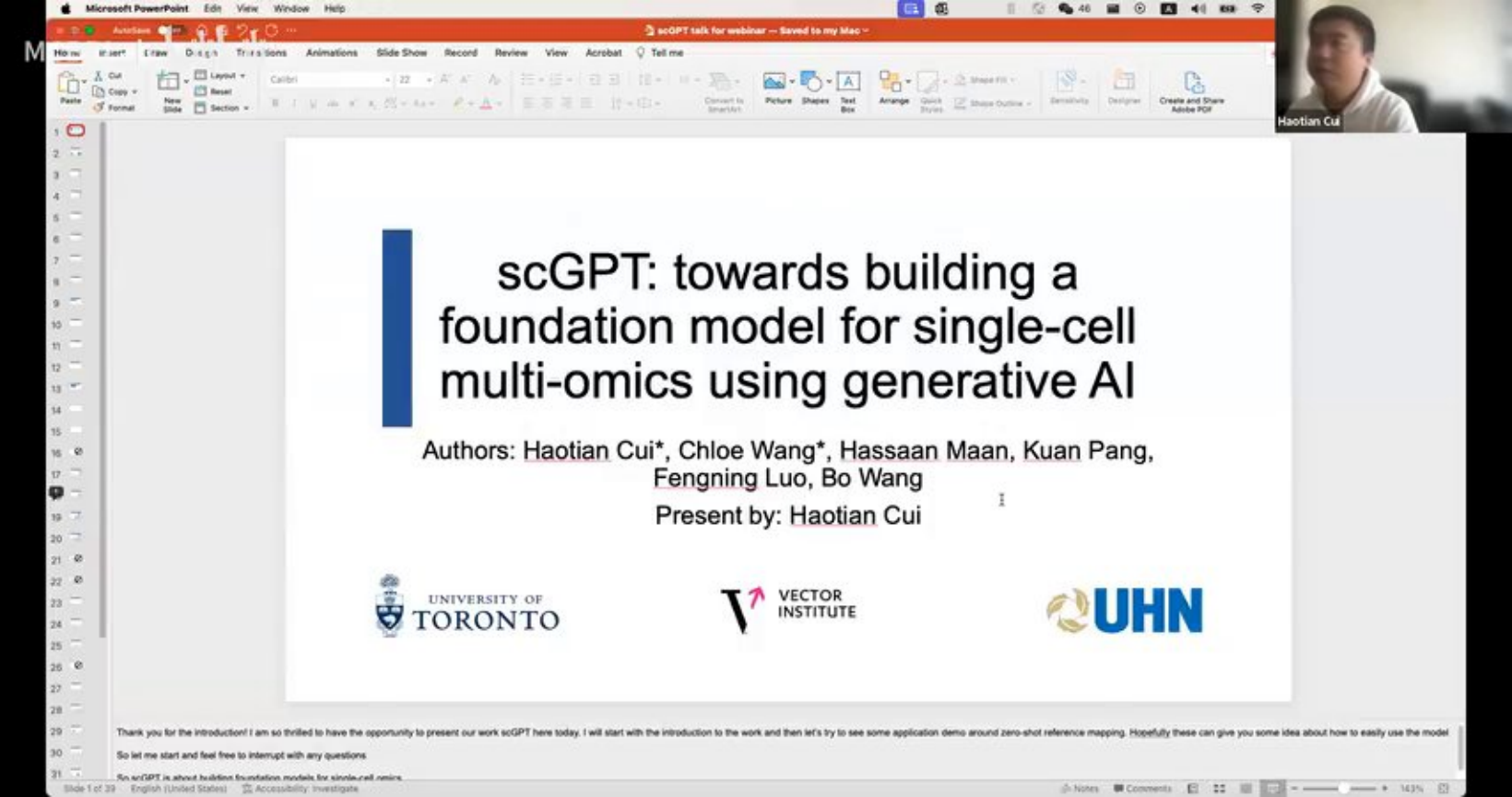
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Thank you for the introduction! I am so thrilled to have the opportunity to present our work scGPT here today. I will start with the introduction to the work and then let's try to see some application demo around zero-shot reference mapping. Hopefully these can give you some idea about how to easily use the model
So let me start and feel free to interrupt with any questions
So scGPT is about building foundation models for single-cell omics

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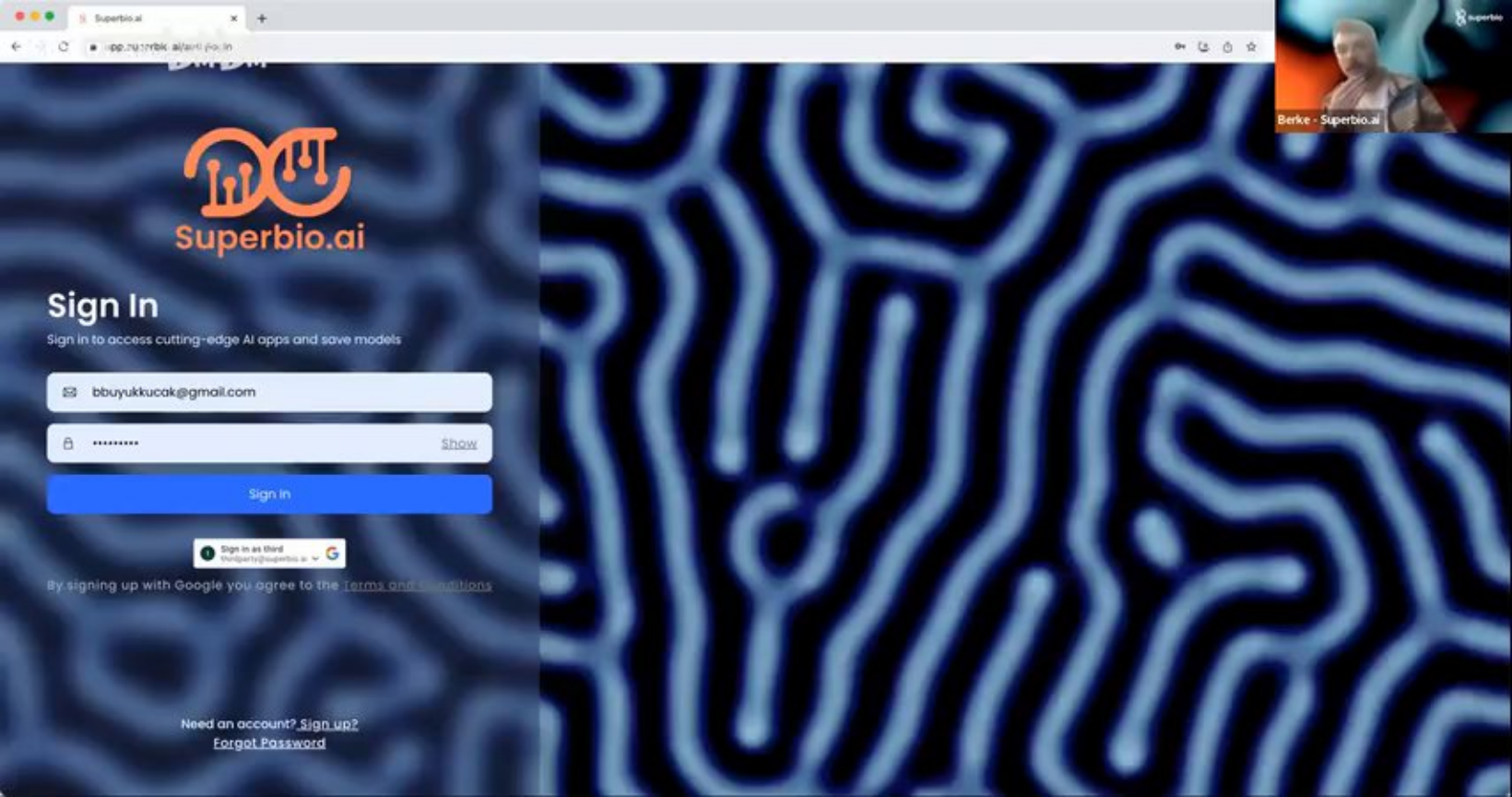
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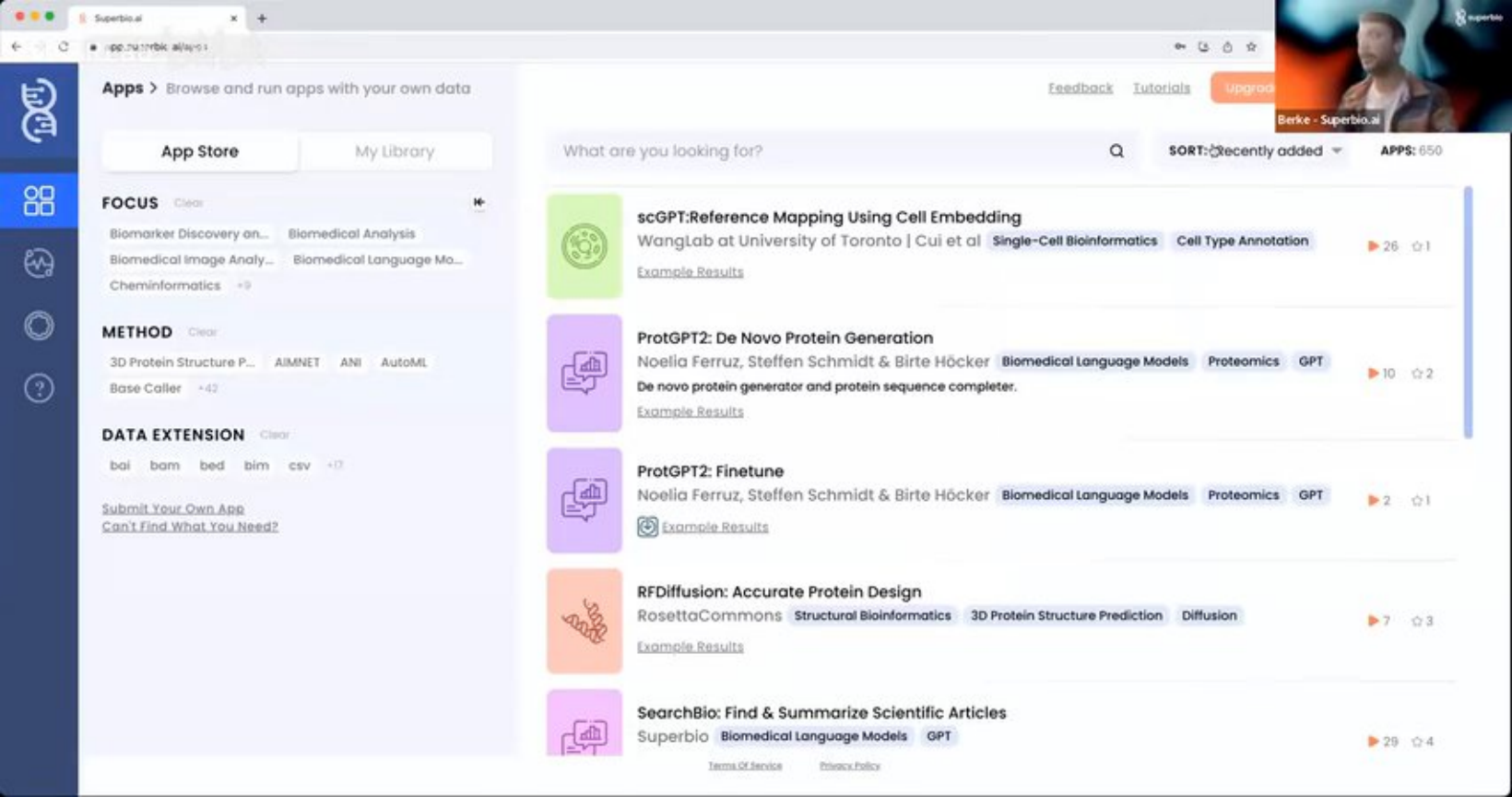
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3D Protein Structure P...
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AutoML
Base Caller
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DATA EXTENSION
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Can't Find What You Need?
scGPT:Reference Mapping Using Cell Embedding
WangLab at University of Toronto | Cui et al
Single-Cell Bioinformatics
Cell Type Annotation
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1
Example Results
ProtGPT2: De Novo Protein Generation
Noelia Ferruz, Steffen Schmidt & Birte Höcker
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De novo protein generator and protein sequence completer.
Example Results
ProtGPT2: Finetune
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1
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RosettaCommons
Structural Bioinformatics
3D Protein Structure Prediction
Diffusion
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Superbio
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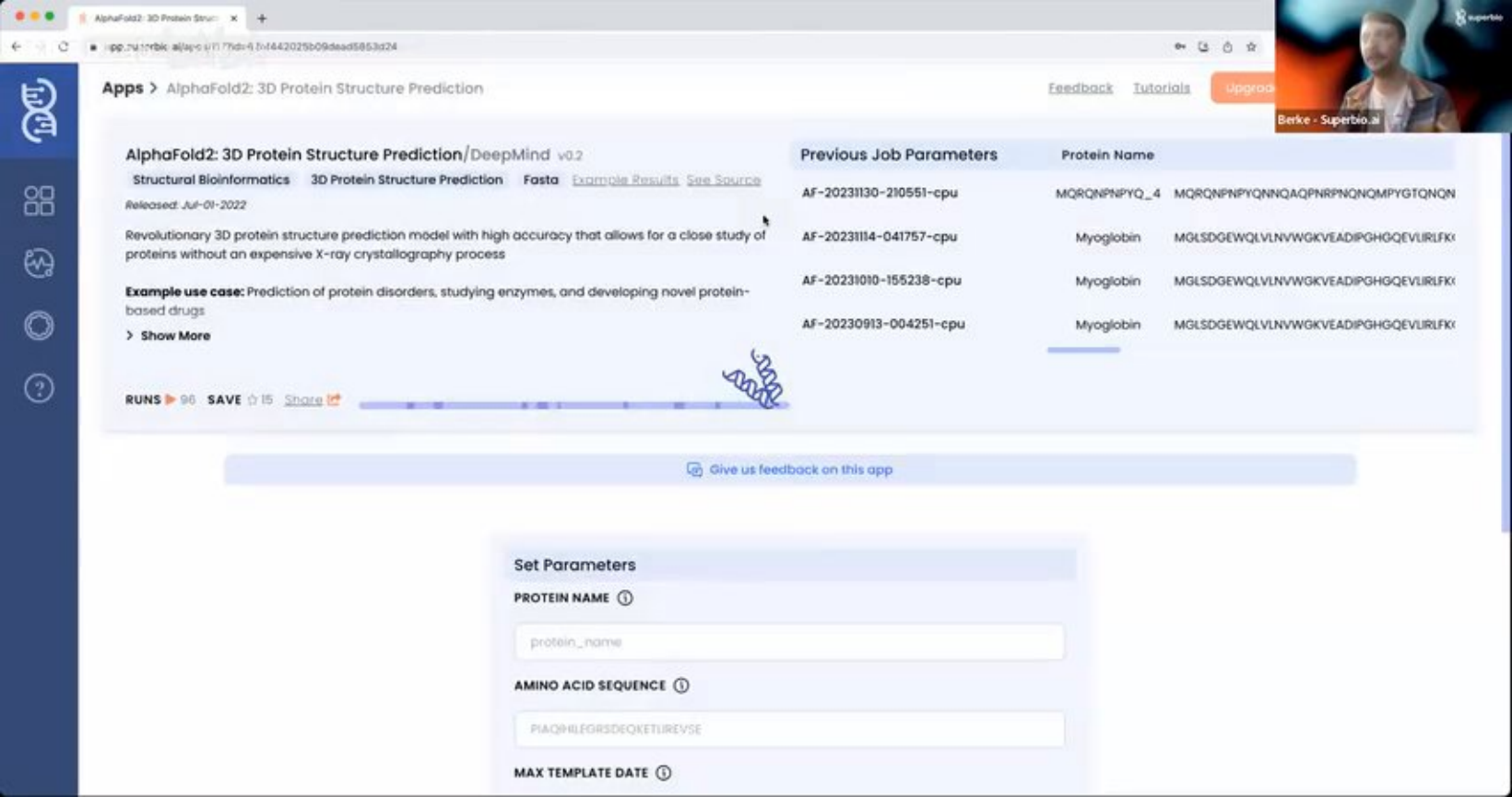
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See Source
Released: Jul-01-2022
Revolutionary 3D protein structure prediction model with high accuracy that allows for a close study of proteins without an expensive X-ray crystallography process
Example use case: Prediction of protein disorders, studying enzymes, and developing novel protein-based drugs
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Protein Name
AF-20231130-210551-cpu
MQRQNPNPYQ_4
MQRQNPNPYQNNQAQPNRPNQNQMPYGTQNQN
AF-20231114-041757-cpu
Myoglobin
MGLSDGEWQLVLNVWGKVEADIPGHGQEVLIRLFK
AF-20231010-155238-cpu
Myoglobin
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AF-20230913-004251-cpu
Myoglobin
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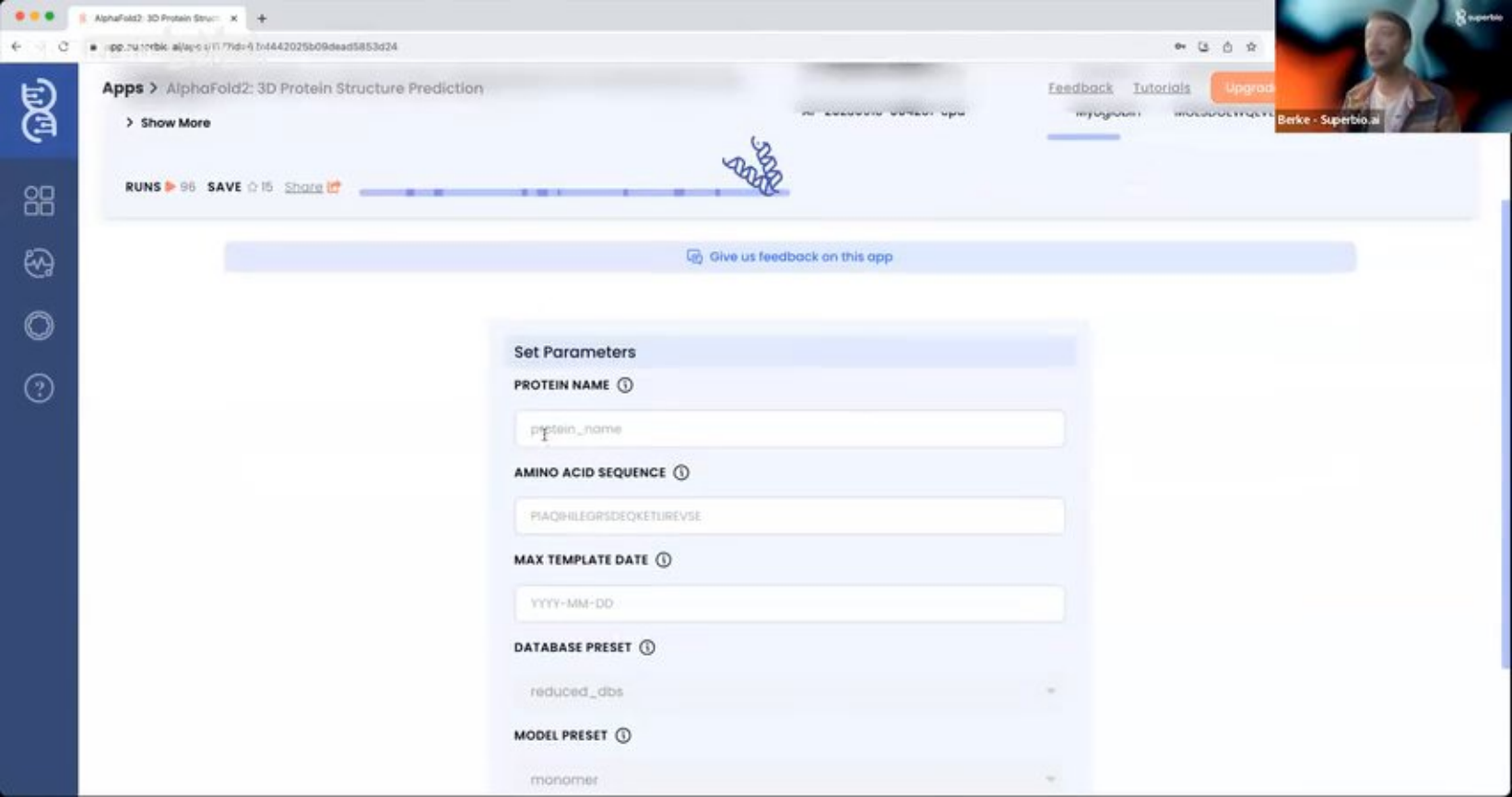
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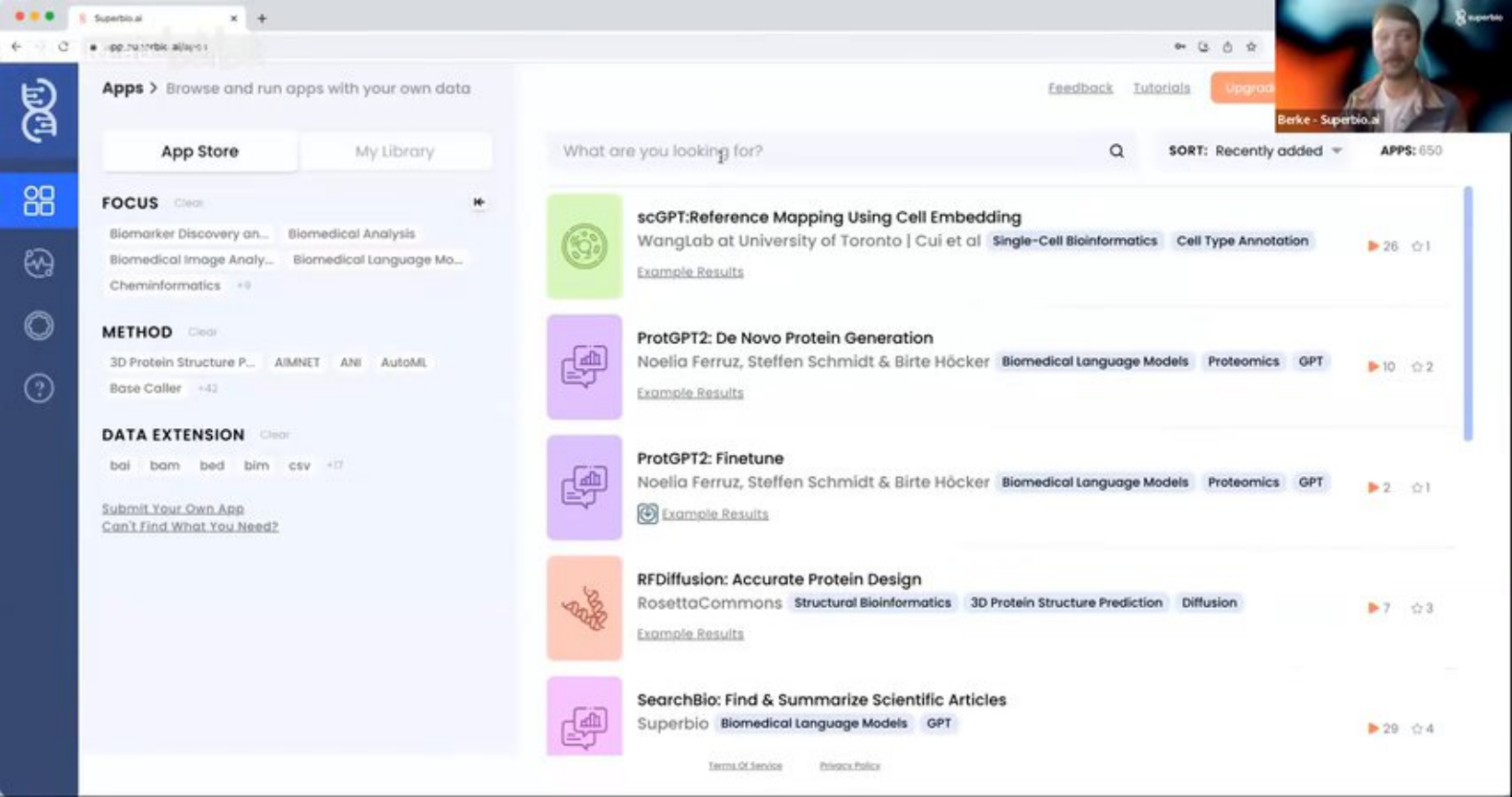
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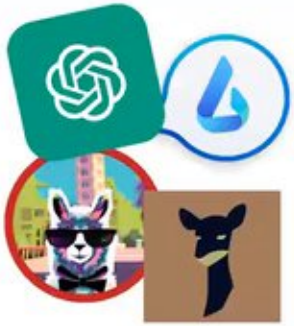
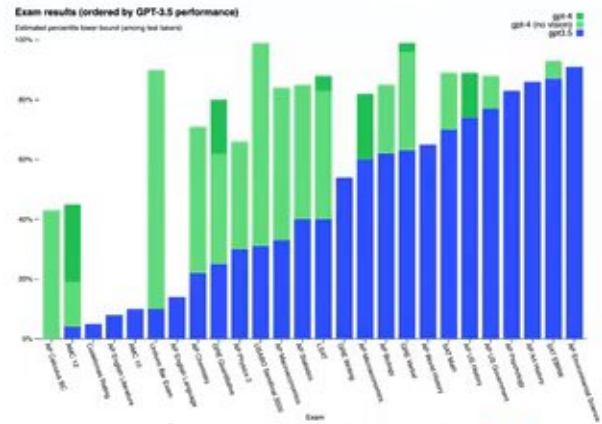
Background of foundation models

- Generative pretraining has achieved remarkable success in various domains such as natural language processing and computer vision
- Specifically, the combination of large-scale diverse datasets and pre-trained transformers has emerged as a promising approach for developing foundation models.

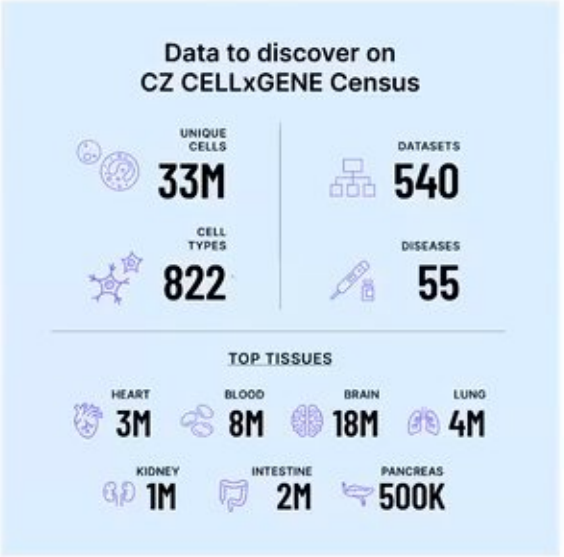




GPT-4 performances on standard exams. Credit to OpenAI

Potential of foundation models for single-cell biol

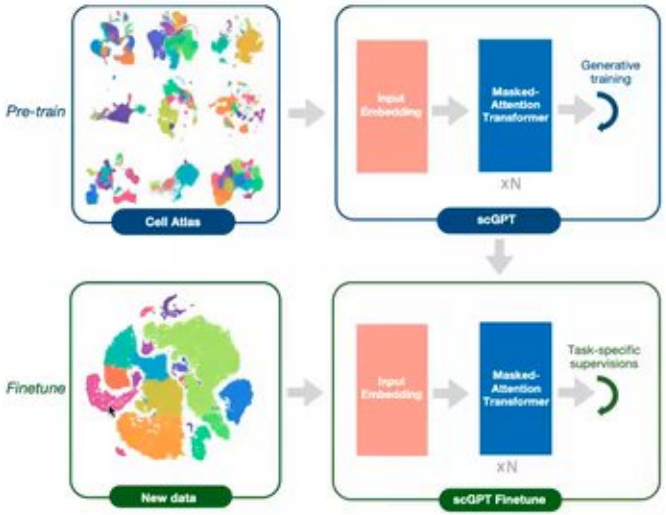
- While texts are made up of words, cells can be characterized by genes.
- This analogy inspires us to explore foundation models for single cell. In the long run, we expect such model has the potential to gain general understanding of molecular biology.
- This is feasible based on two considerations:
  - Transformers would a suitable to learn interactions between gene tokens.
  - The vast scale of sequencing data, of diverse cell types and conditions, and it is growing exponentially.



We are particularly excited about the recent launch of CellxGene census. Figure credit to @JCoolScience

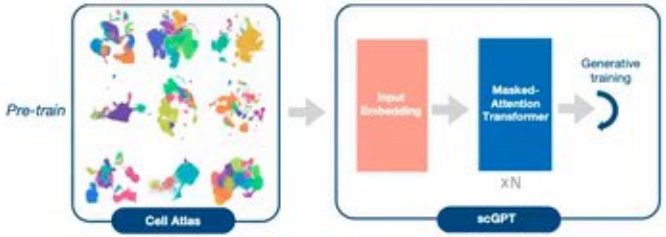
Overview of scGPT

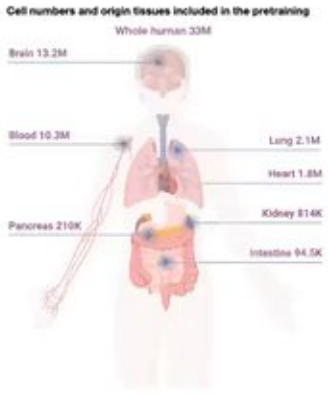
- We present scGPT to construct a single-cell foundation model. The workflow contains two steps:
  1. Generative **pre-training** on over 33 million normal human cells
  2. **Fine-tuning** for downstream tasks



Generative pretraining in scGPT

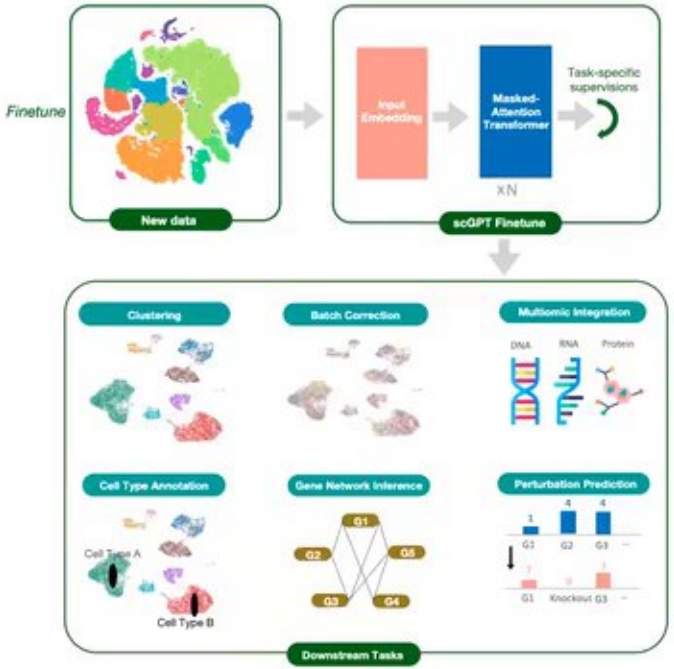
- In the pre-training:
  - Large-scale expression matrices were collected and preprocessed
  - We selected around 33 million normal human cells of 51 organs/tissues from the CZ CellxGene collection
  - Numbers of cells from major tissues shown on the right





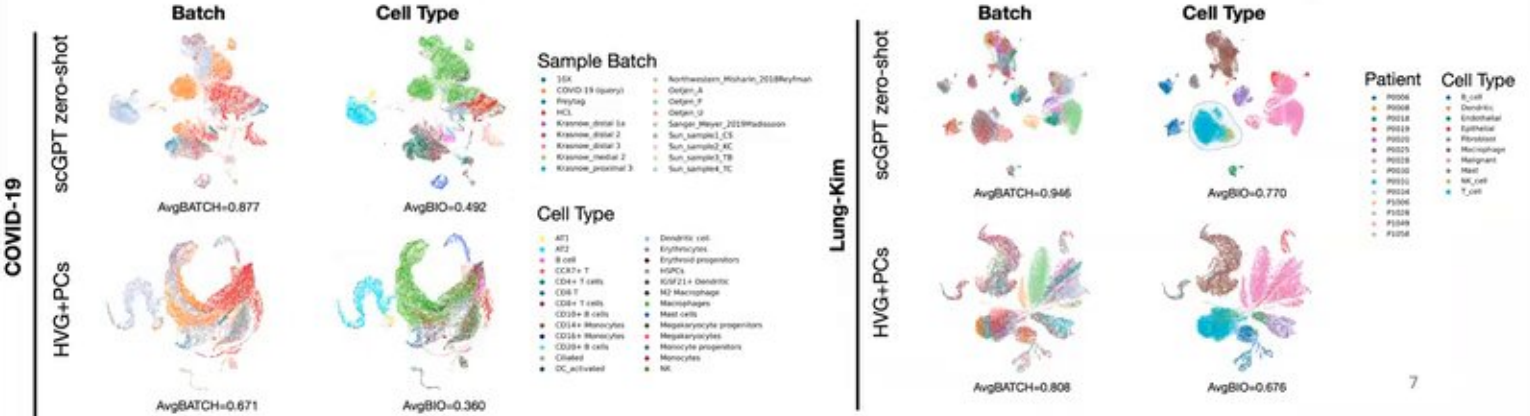
Overview of fine-tuning in scGPT

- In fine-tuning:
  - A set of versatile learning objectives are adopted to readily support various applications
  - Self-supervised objectives:
    - Gene Expression Prediction (GEP)
    - Gene Expression Prediction for Cell Modelling (GEPC)
    - Elastic Cell Similarity (ECS)
  - Supervised objectives:
    - Domain Adaptation via Reverse Back-propagation (DAR)
    - Cell Type Classification (CLS)



Zero-shot applications

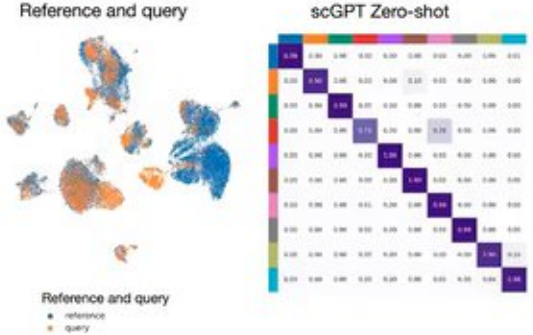
- **Zero-shot**, meaning using the pretrained model to generate embeddings for new data, without any further training, **much faster, more accessible**
- UMAP of zero-shot embeddings on two disease datasets, compared to HVGs
  - Considerable ability to distinguish cell types
  - Note the pretraining process is not designed for mitigating technical batch effects



Zero-shot reference mapping

- We also use the embeddings in a reference mapping manner
- We split the data to simulate a setting that some of the patient cells, query set, were not annotated. Cell types were propagated from reference data set to label the query set.
- The zero-shot workflow demonstrates competitive accuracy across comparisons.

Lung-Kim



Dataset	Method	Evaluation Metrics			
		Accuracy	*Precision*	*Recall*	*MacroF1*
COVID-19	scGPT (fine-tuned)	**0.891**	**0.577**	**0.567**	**0.547**
	scGPT (zero-shot)	0.867	0.513	0.476	0.468
	Azimuth	0.878	0.515	0.418	0.444
	expiMap	0.730	0.441	0.325	0.335
Lung-Kim	scGPT (fine-tuned)	**0.974**	0.959	**0.967**	**0.962**
	scGPT (zero-shot)	0.968	**0.970**	0.933	0.948
	Azimuth	0.970	0.957	0.962	0.959
	expiMap	0.920	0.940	0.846	0.878

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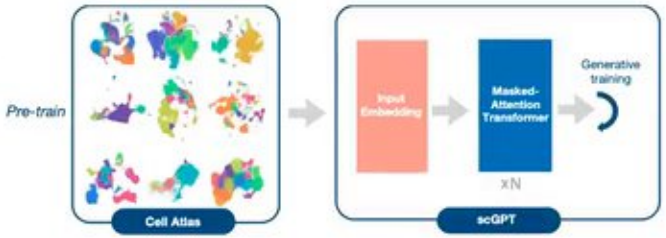

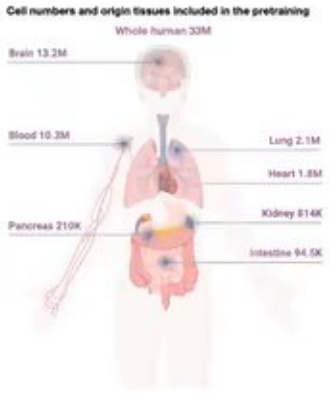

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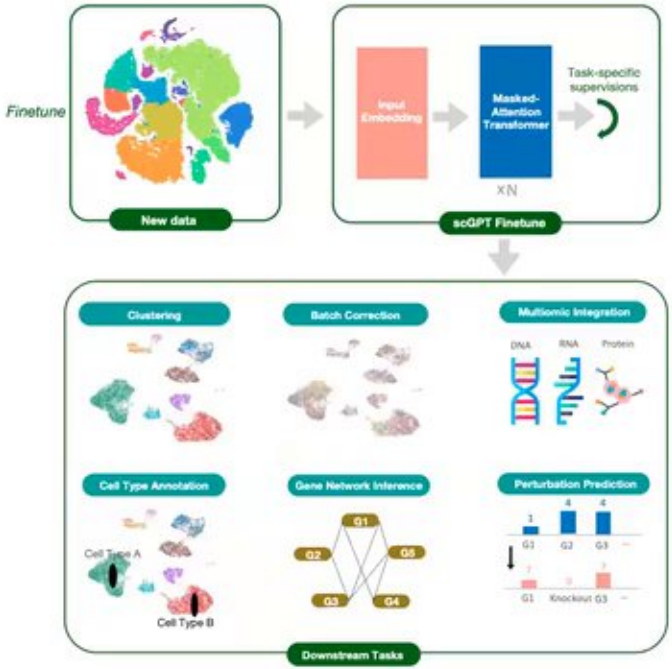

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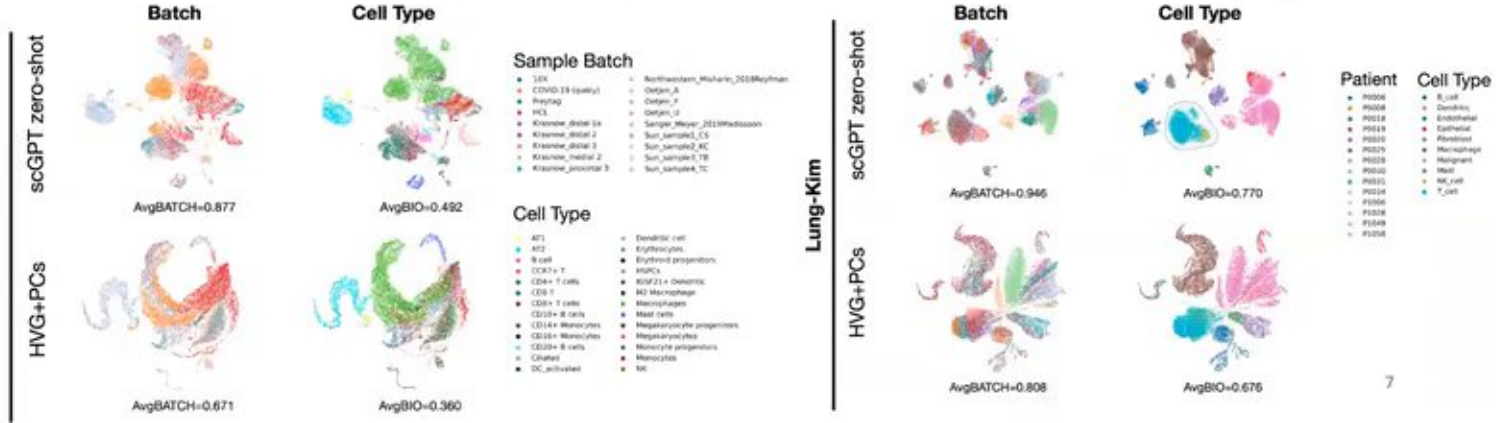

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Zero-shot ref map to cell atlas

- Zero-shot embeddings can further be used to map cells and propagate metainfo from large cell atlas
- For this new feature, we generated the cell embeddings for millions of cells on CellXGene, and build an index for efficient similarity search using the faiss toolbox.
- This can be used to query new cells super fast, https://github.com/bowang-lab/scGPT/blob/main/tutorials/Tutorial_Reference_Mapping.ipynb

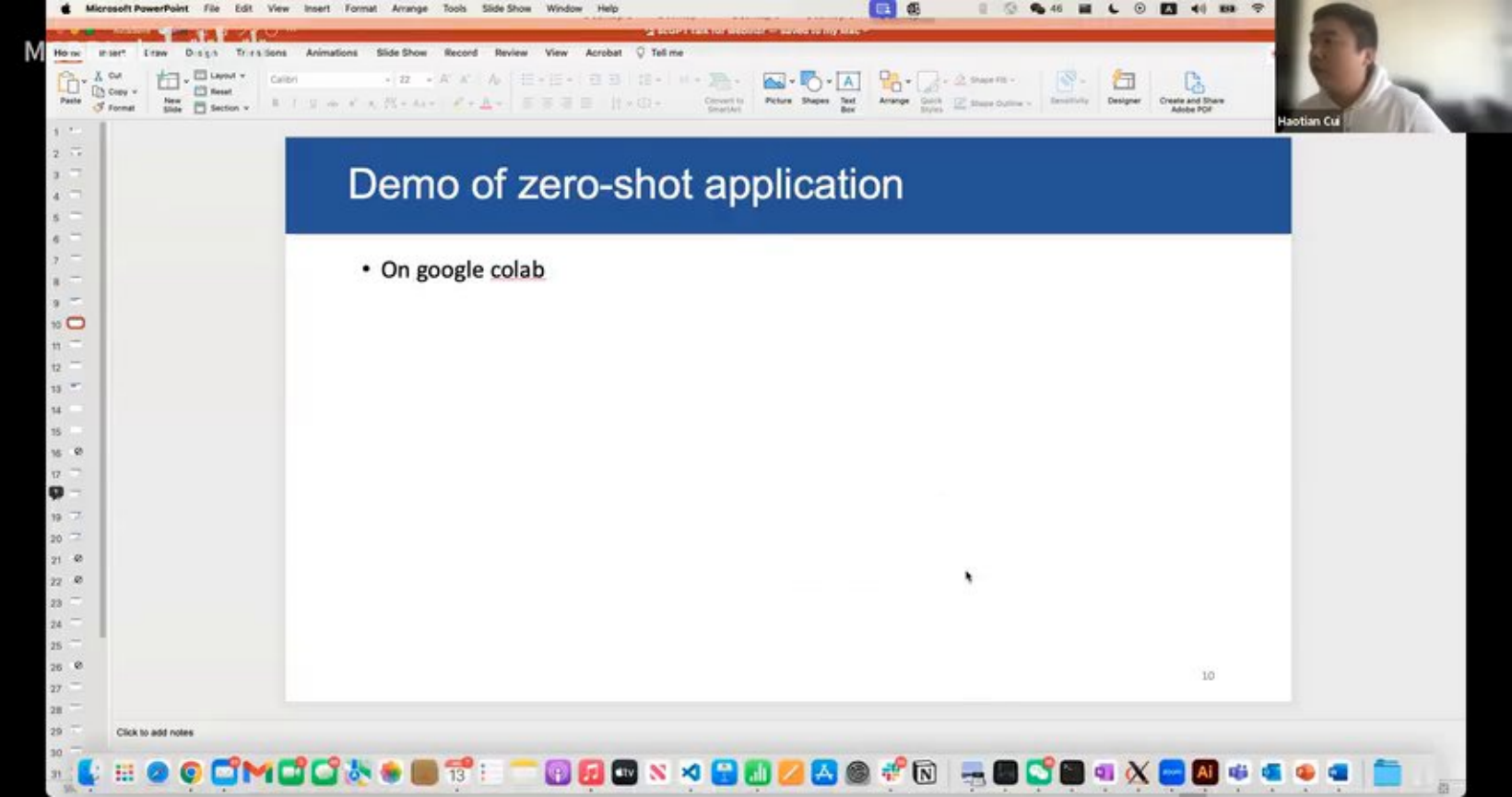
The search runs super fast, especially on GPU. Here the similarity search for 4,000 query cells within the whole reference of millions should take around 7 second on CPU and 0.1 second on GPU.

In [10]:
```
%%time
k = 50
# test with the first 100 cells
distances, idx = index.search(test_emebd, k)
```

```
CPU times: user 252 ms, sys: 493 ms, total: 745 ms
Wall time: 133 ms
```

Demo of zero-shot application

- On google colab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Demo of zero-shot application
• On google colab
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Zero-shot reference mapping tutorial with scGPT

Introduction

This tutorial covers the zero-shot reference mapping with scGPT. This workflow achieves accurate and fast reference mapping for scRNA-seq datasets without fine-tuning (or any extensive training) of scGPT. To further boost the performance, we recommend fine-tuning scGPT.

We will use COVID-19 dataset to demonstrate the zero-shot reference mapping. You can download the processed reference and query datasets from here. The COVID-19 dataset is derived from the work by Lotfollahi et al, which contains 18 distinct batches and diverse samples from lung tissues. The reference dataset consists of 15,997 cells and the query dataset contains 4,003 cells. You may place the dataset under `data` directory in the outer level.

Particularly, we use the `scGPT_human` model to provide embeddings out of the box. You may download it from here.

The zero-shot reference mapping workflow is as follows:

1. Load and pre-process the dataset
2. Generate scGPT embeddings for each cell in reference and query datasets
3. Transfer the annotations from reference to query dataset

At the appendix of this tutorial, we will also showcase the zero-shot reference mapping on Lung dataset. You can find the dataset here.

We use a similarity-based method for transferring the annotation, which involves comparing the similarity between the query cell embedding and the reference cell embeddings. We use FAISS to perform the similarity search.

Open in Colab

[1] # Specifically for Google Colab, install dependencies and download data

```
import os
import sys

if "google.colab" in sys.modules:
    print("Running on Google Colab")
    print("Installing dependencies...")
    !pip install -U scgpt
```

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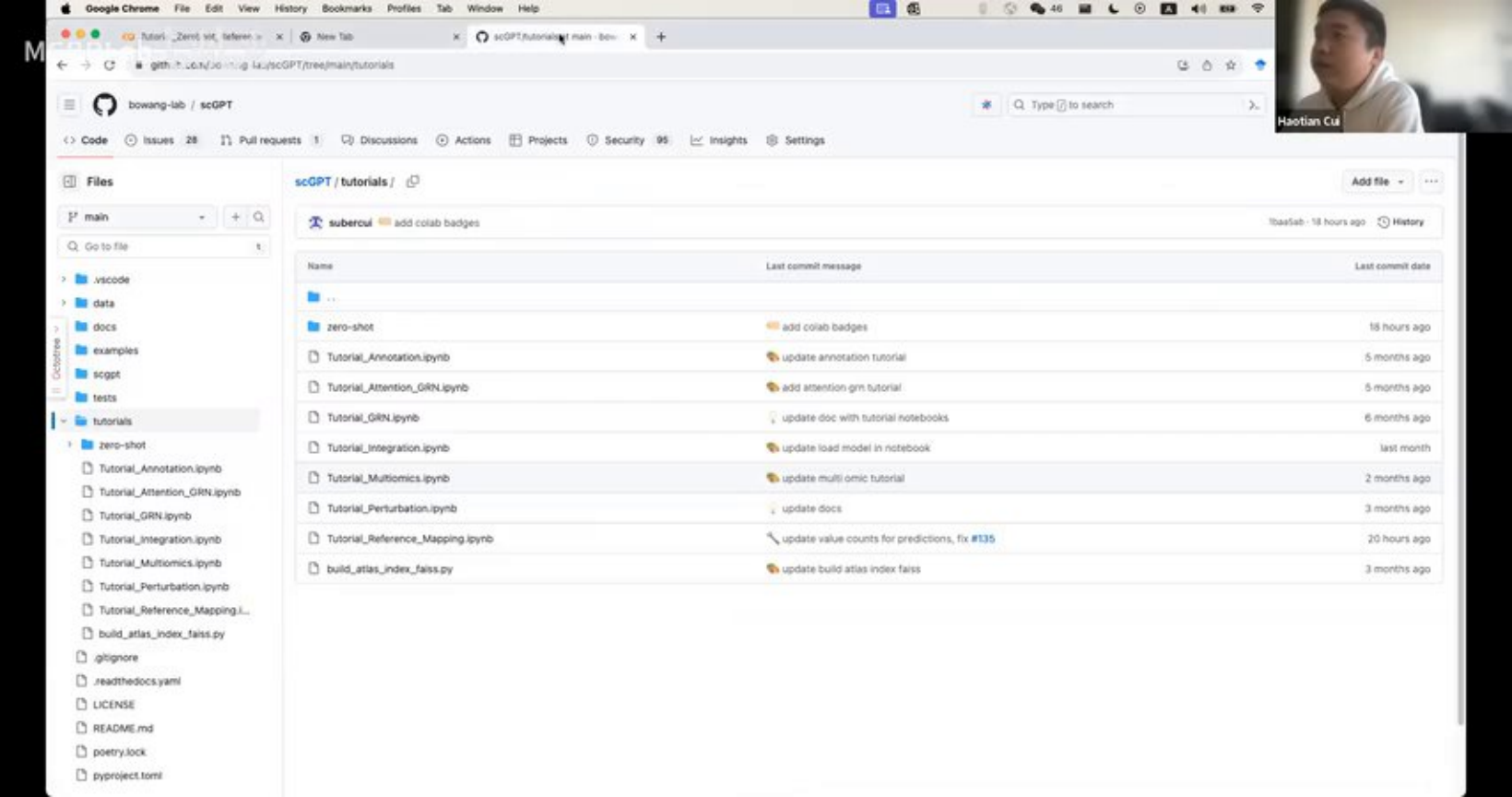
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Tutorial_Integration.ipynb
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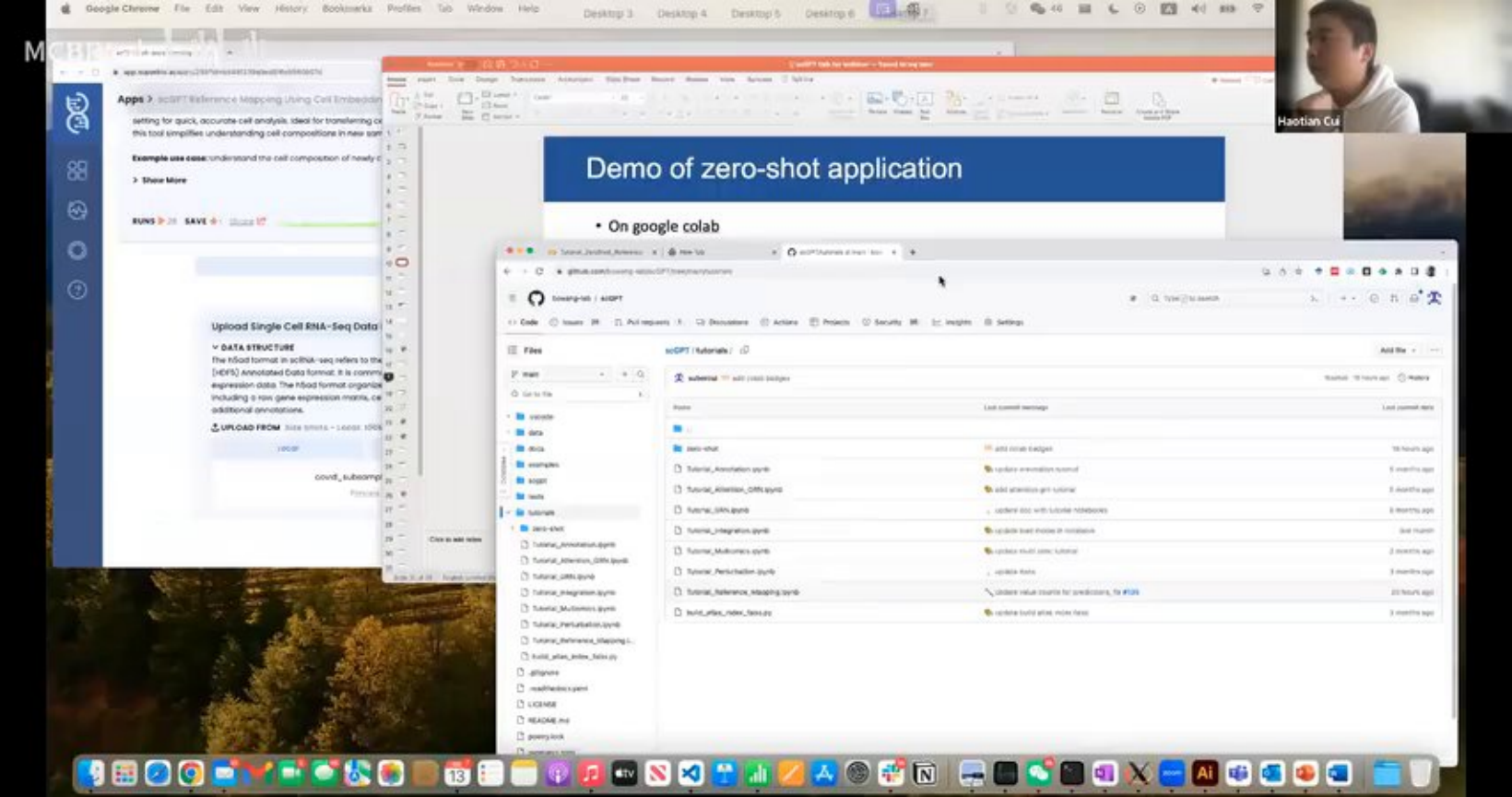
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Demo of zero-shot application
• On google colab

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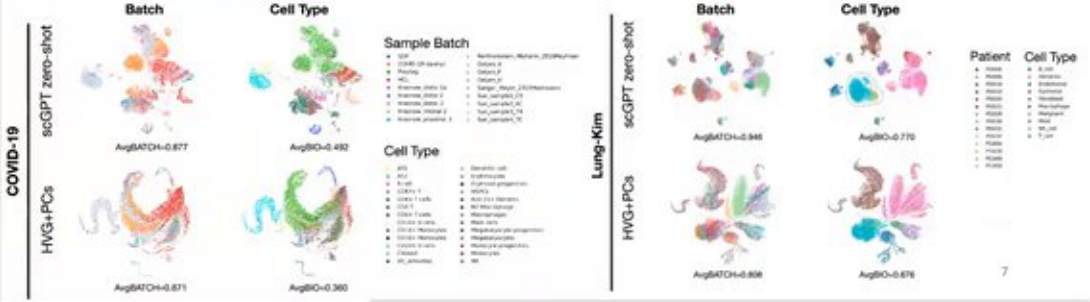
Zero-shot applications

- **Zero-shot**, meaning using the pretrained model to generate embeddings for new data, without any further training, **much faster, more accessible**
- UMAP of zero-shot embeddings on two disease datasets, compared to HVGs
  - Considerable ability to distinguish cell types
  - Note the pretraining process is not designed for mitigating technical batch effects

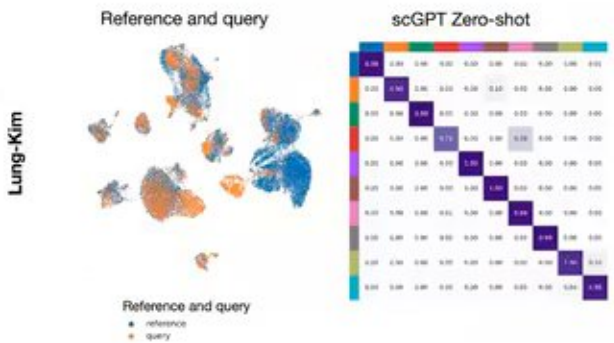


Have been working new extensions exploring the possibility of zero-shot applications. Here, I'd like to share some new results

Particularly want to mention the influence of pretraining,
so of the technical info is actually signals

Zero-shot reference mapping

- We also use the embeddings in a reference mapping manner
- We split the data to simulate a setting that some of the patient cells, query set, were not annotated. Cell types were propagated from reference data set to label the query set.
- The zero-shot workflow demonstrates competitive accuracy across comparisons.



Dataset	Method	Evaluation Metrics			
		Accuracy	*Precision*	*Recall*	*MacroF1*
COVID-19	scGPT (fine-tuned)	**0.891**	**0.577**	**0.567**	**0.547**
	scGPT (zero-shot)	0.867	0.513	0.476	0.468
	Azimuth	0.878	0.515	0.418	0.444
	expiMap	0.730	0.441	0.325	0.335
Lung-Kim	scGPT (fine-tuned)	**0.974**	0.959	**0.967**	**0.962**
	scGPT (zero-shot)	0.968	**0.970**	0.933	0.948
	Azimuth	0.970	0.957	0.962	0.959
	expiMap	0.920	0.940	0.846	0.878

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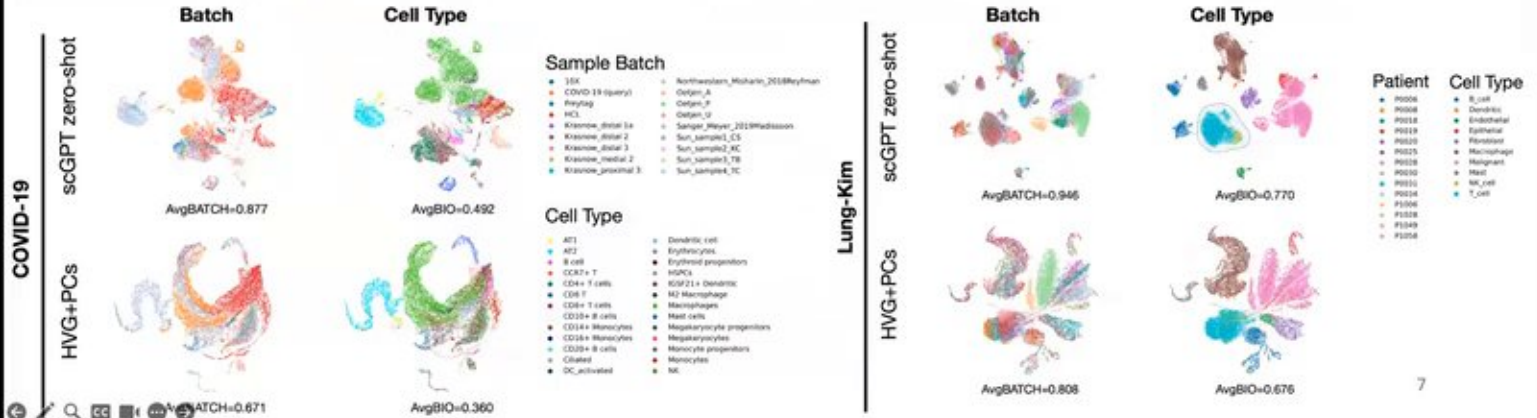

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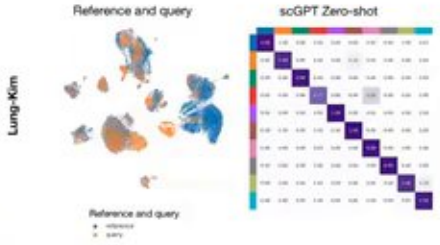

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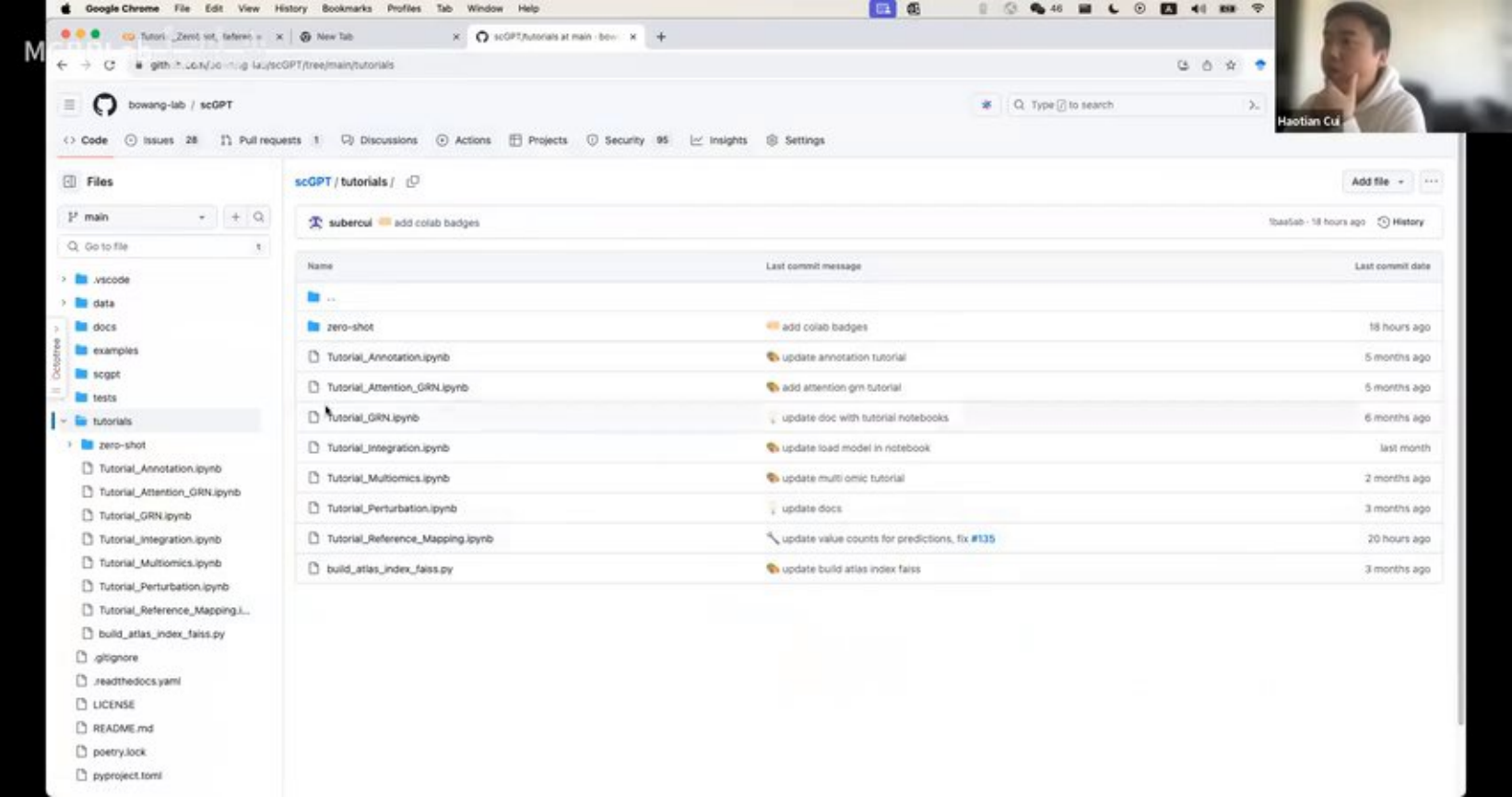
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6 months ago
Tutorial_Integration.ipynb
update load model in notebook
last month
Tutorial_Multiomics.ipynb
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2 months ago
Tutorial_Perturbation.ipynb
update docs
3 months ago
Tutorial_Reference_Mapping.ipynb
update value counts for predictions, fix #135
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3 months ago
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main

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  - Tutorial_Attention_GRN.ipynb
  - Tutorial_GRN.ipynb
  - Tutorial_Integration.ipynb
  - Tutorial_Multiomics.ipynb
  - Tutorial_Perturbation.ipynb
  - Tutorial_Reference_Mapping.i...
  - build_atlas_index_faiss.py
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- .readthedocs.yaml
- LICENSE
- README.md
- poetry.lock
- pyproject.toml

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Zero-shot reference mapping tutorial with scGPT

Introduction

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Open in Colab

In [1]:

```
# Specifically for Google Colab, install dependencies and download data

import os
import sys

if "google.colab" in sys.modules:
    print("Running on Google Colab")
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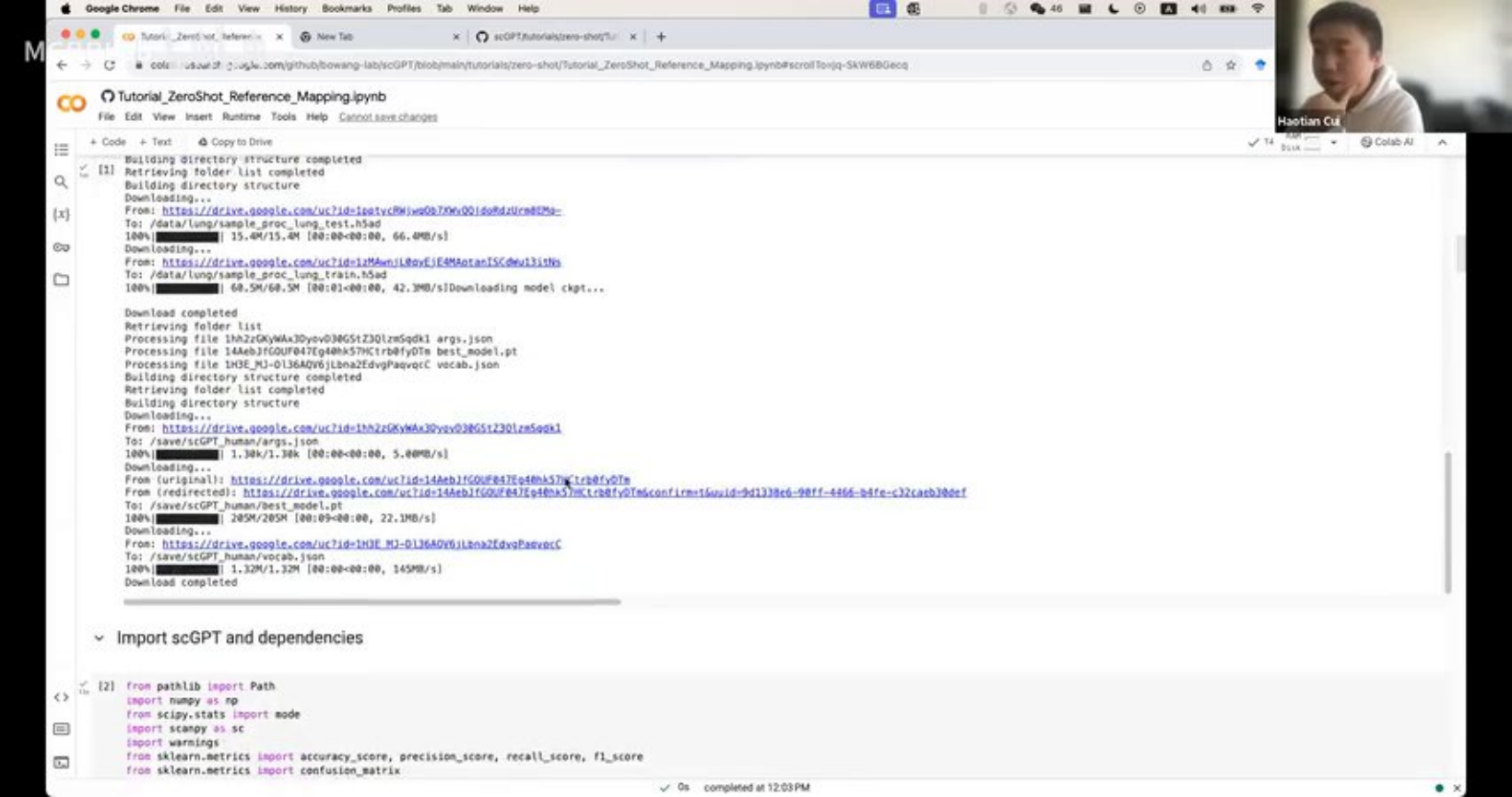
    !pip install -U scgpt
    # the optional dependency of flash-attion is skipped on colab
    !pip install wandb louvain faiss-cpu

    # NOTE: May need to restart runtime after the installation
```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Building directory structure completed
Retrieving folder list completed
Building directory structure
Downloading...
From: https://drive.google.com/uc?id=1patycRWjwqOb7XWvQQ1doRdzUrm8EMa-
To: /data/lung/sample_proc_lung_test.h5ad
100%| | 15.4M/15.4M [00:00<00:00, 66.4MB/s]
Downloading...
From: https://drive.google.com/uc?id=1zMAwnjL8qvEjE4MAotanISCdWu13itNs
To: /data/lung/sample_proc_lung_train.h5ad
100%| | 60.5M/60.5M [00:01<00:00, 42.3MB/s]Downloading model ckpt...
Download completed
Retrieving folder list
Processing file 1hh2zGKyWAx3OyovO30GStZ3QlzmSqdk1 args.json
Processing file 14AebJfGOUF047Eg40hk57HCtrb0fyDTm best_model.pt
Processing file 1H3E_MJ-Dl36AQV6jLbna2EdvgPaqvqcC vocab.json
Building directory structure completed
Retrieving folder list completed
Building directory structure
Downloading...
From: https://drive.google.com/uc?id=1hh2zGKyWAx3OyovO30GStZ3QlzmSqdk1
To: /save/scGPT_human/args.json
100%| | 1.30k/1.30k [00:00<00:00, 5.00MB/s]
Downloading...
From (original): https://drive.google.com/uc?id=14AebJfGOUF047Eg40hk57HCtrb0fyDTm
From (redirected): https://drive.google.com/uc?id=14AebJfGOUF047Eg40hk57HCtrb0fyDTm&confirm=t&uuid=9d1338e6-90ff-4466-b4fe-c32caeb300ef
To: /save/scGPT_human/best_model.pt
100%| | 205M/205M [00:09<00:00, 22.1MB/s]
Downloading...
From: https://drive.google.com/uc?id=1H3E_MJ-Dl36AQV6jLbna2EdvgPaqvqcC
To: /save/scGPT_human/vocab.json
100%| | 1.32M/1.32M [00:00<00:00, 145MB/s]
Download completed
Import scGPT and dependencies
[2] from pathlib import Path
import numpy as np
from scipy.stats import mode
import scanpy as sc
import warnings
from sklearn.metrics import accuracy_score, precision_score, recall_score, f1_score
from sklearn.metrics import confusion_matrix
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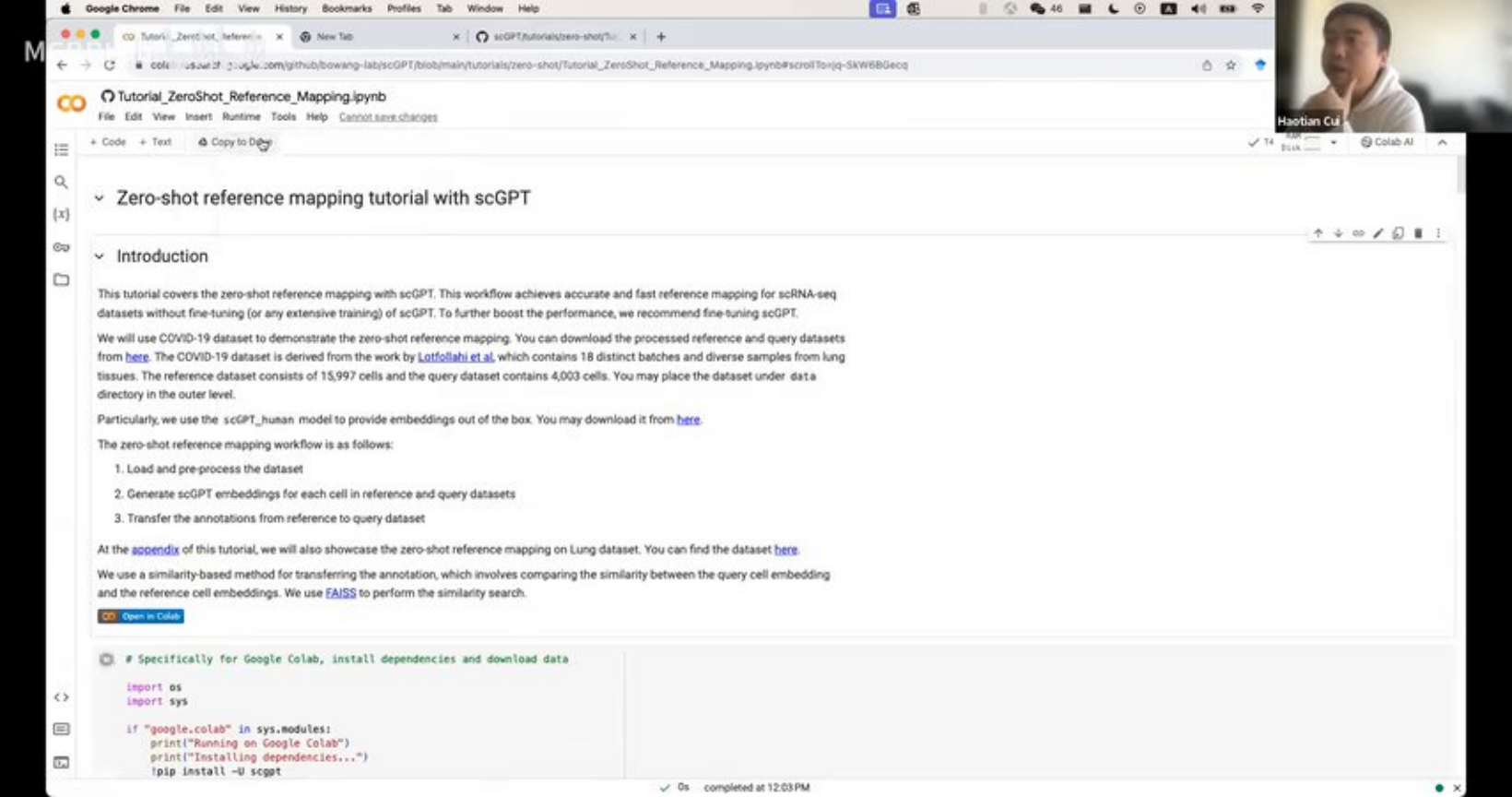
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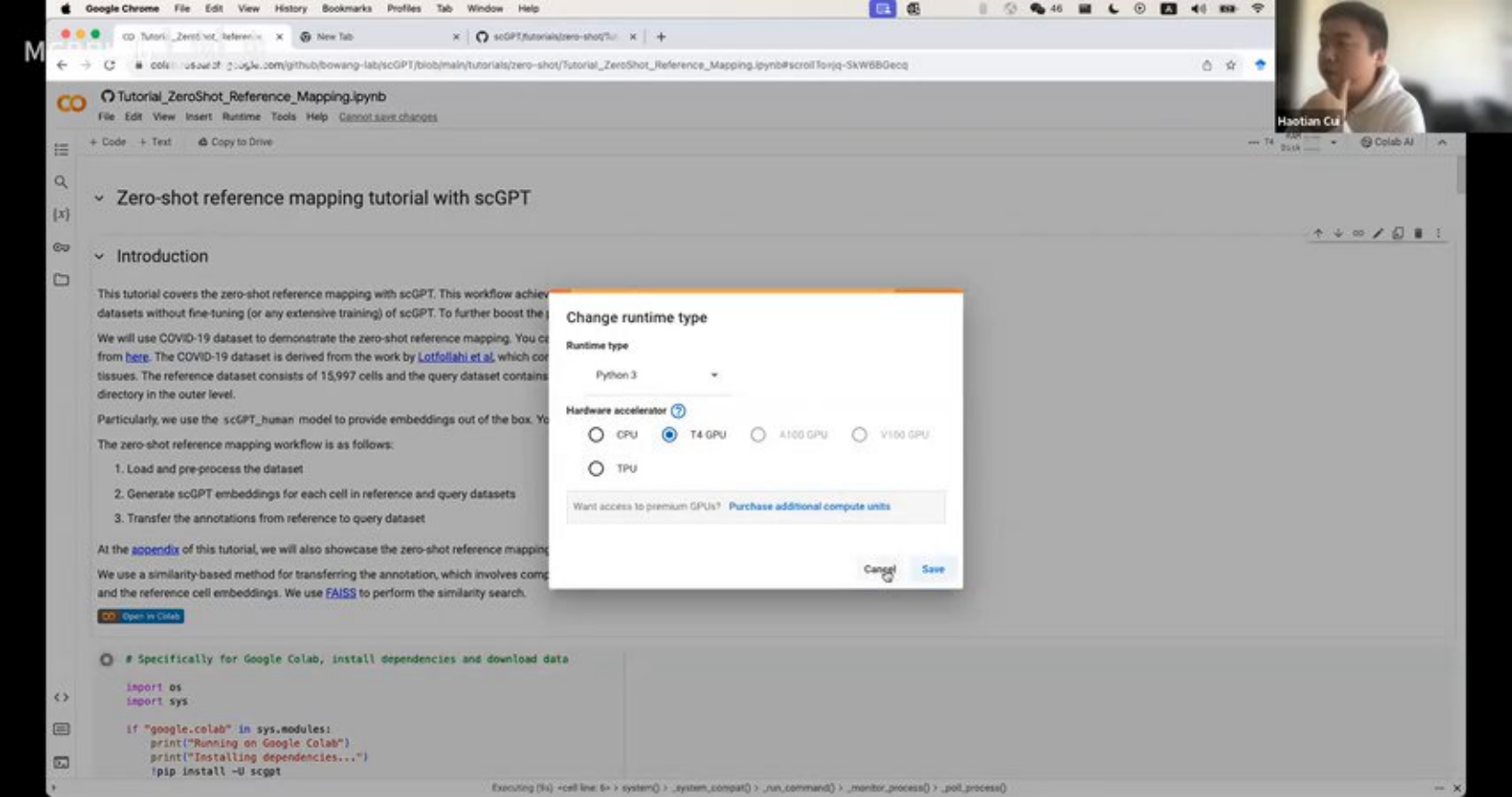
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Change runtime type
Runtime type
Python 3
Hardware accelerator
CPU T4 GPU A100 GPU V100 GPU
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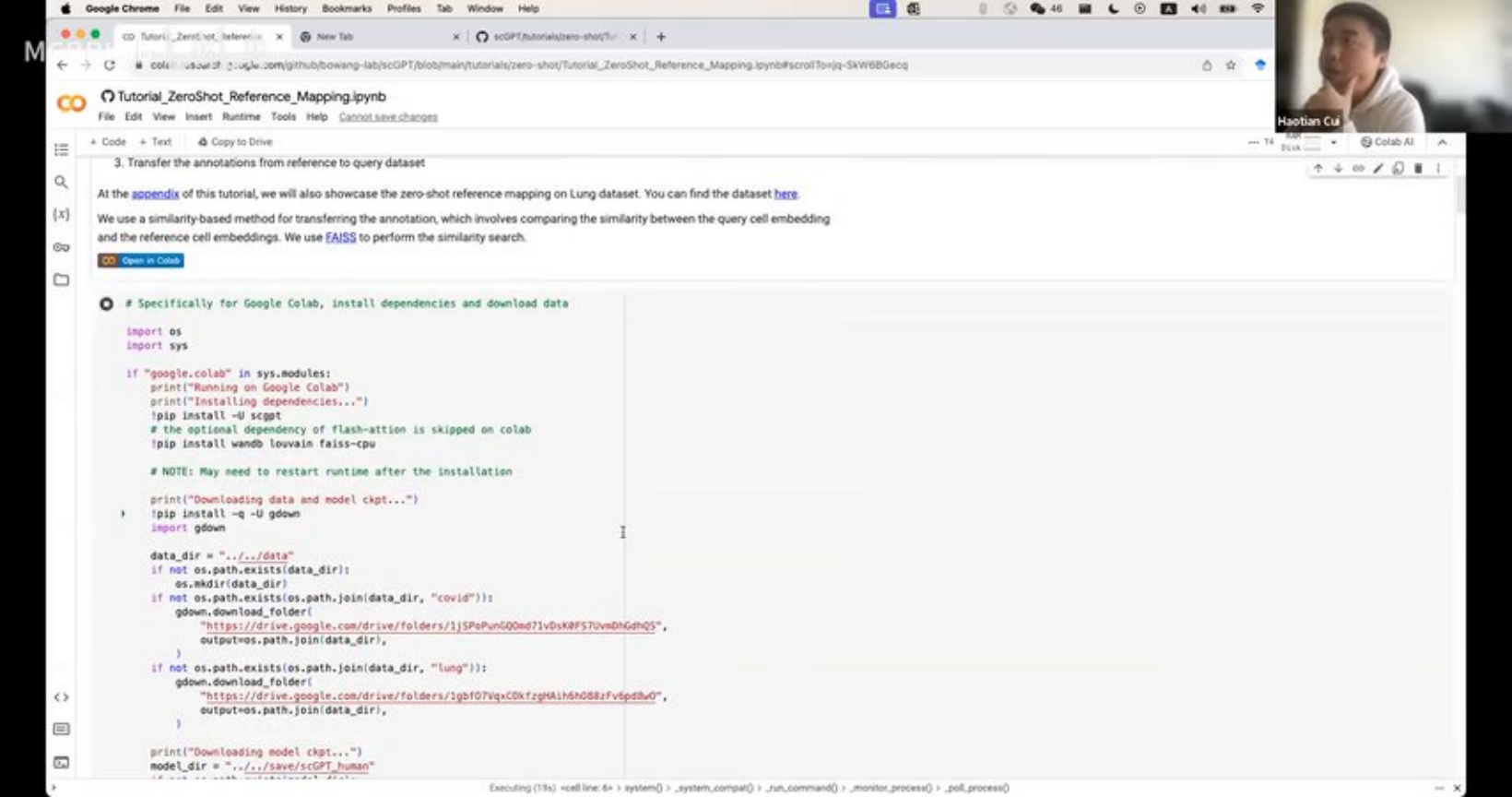
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!pip install -q -U gdown
import gdown
data_dir = "../../data"
if not os.path.exists(data_dir):
os.mkdir(data_dir)
if not os.path.exists(os.path.join(data_dir, "covid")):
gdown.download_folder(
"https://drive.google.com/drive/folders/1jSPoPunGQOmd71vDsK0FS7UvmDhGdhQS",
output=os.path.join(data_dir),
)
if not os.path.exists(os.path.join(data_dir, "lung")):
gdown.download_folder(
"https://drive.google.com/drive/folders/1gbfG7VqxC0kfzgHAih6hO88zFv6pd8wO",
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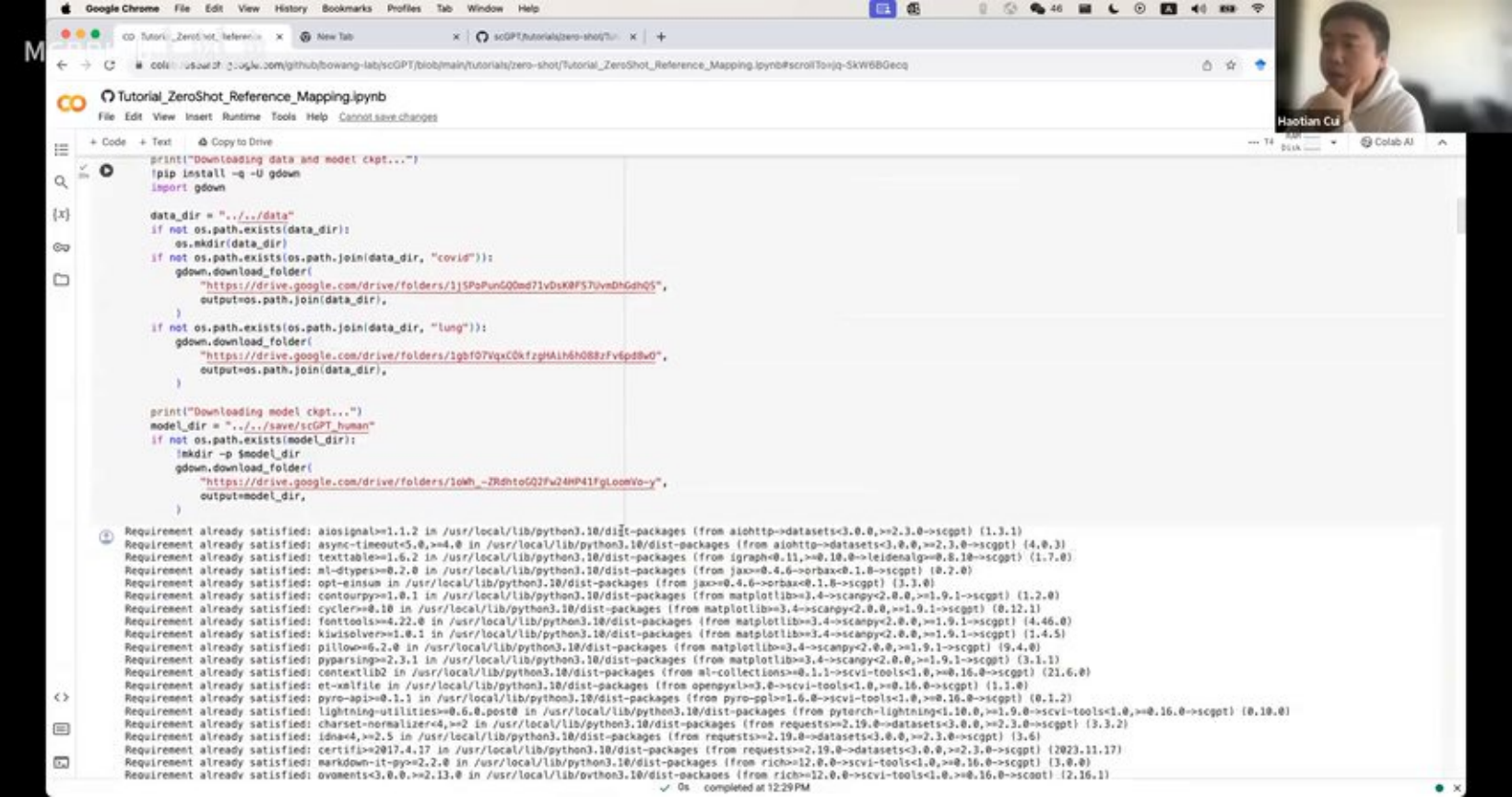
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output=model_dir,
)
Requirement already satisfied: aiosignal>=1.1.2 in /usr/local/lib/python3.10/dist-packages (from aiohttp->datasets<3.0.0,>=2.3.0->scgpt) (1.3.1)
Requirement already satisfied: async-timeout<5.0,>=4.0 in /usr/local/lib/python3.10/dist-packages (from aiohttp->datasets<3.0.0,>=2.3.0->scgpt) (4.0.3)
Requirement already satisfied: texttable>=1.6.2 in /usr/local/lib/python3.10/dist-packages (from igraph<0.11,>=0.10.0->leidenalg>=0.8.10->scgpt) (1.7.0)
Requirement already satisfied: ml-dtypes>=0.2.0 in /usr/local/lib/python3.10/dist-packages (from jax>=0.4.6->orbax<0.1.8->scgpt) (0.2.0)
Requirement already satisfied: opt-einsum in /usr/local/lib/python3.10/dist-packages (from jax>=0.4.6->orbax<0.1.8->scgpt) (3.3.0)
Requirement already satisfied: contourpy>=1.0.1 in /usr/local/lib/python3.10/dist-packages (from matplotlib>=3.4->scanpy<2.0.0,>=1.9.1->scgpt) (1.2.0)
Requirement already satisfied: cycler>=0.10 in /usr/local/lib/python3.10/dist-packages (from matplotlib>=3.4->scanpy<2.0.0,>=1.9.1->scgpt) (0.12.1)
Requirement already satisfied: fonttools>=4.22.0 in /usr/local/lib/python3.10/dist-packages (from matplotlib>=3.4->scanpy<2.0.0,>=1.9.1->scgpt) (4.46.0)
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Requirement already satisfied: pyro-api>=0.1.1 in /usr/local/lib/python3.10/dist-packages (from pyro-ppl>=1.6.0->scvi-tools<1.0,>=0.16.0->scgpt) (0.1.2)
Requirement already satisfied: lightning-utilities>=0.6.0.post0 in /usr/local/lib/python3.10/dist-packages (from pytorch-lightning<1.10.0,>=1.9.0->scvi-tools<1.0,>=0.16.0->scgpt) (0.10.0)
Requirement already satisfied: charset-normalizer<4,>=2 in /usr/local/lib/python3.10/dist-packages (from requests>=2.19.0->datasets<3.0.0,>=2.3.0->scgpt) (3.3.2)
Requirement already satisfied: idna<4,>=2.5 in /usr/local/lib/python3.10/dist-packages (from requests>=2.19.0->datasets<3.0.0,>=2.3.0->scgpt) (3.6)
Requirement already satisfied: certifi>=2017.4.17 in /usr/local/lib/python3.10/dist-packages (from requests>=2.19.0->datasets<3.0.0,>=2.3.0->scgpt) (2023.11.17)
Requirement already satisfied: markdown-it-py>=2.2.0 in /usr/local/lib/python3.10/dist-packages (from rich>=12.0.0->scvi-tools<1.0,>=0.16.0->scgpt) (3.0.0)
Requirement already satisfied: pygments<3.0.0,>=2.13.0 in /usr/local/lib/python3.10/dist-packages (from rich>=12.0.0->scvi-tools<1.0,>=0.16.0->scgpt) (2.16.1)
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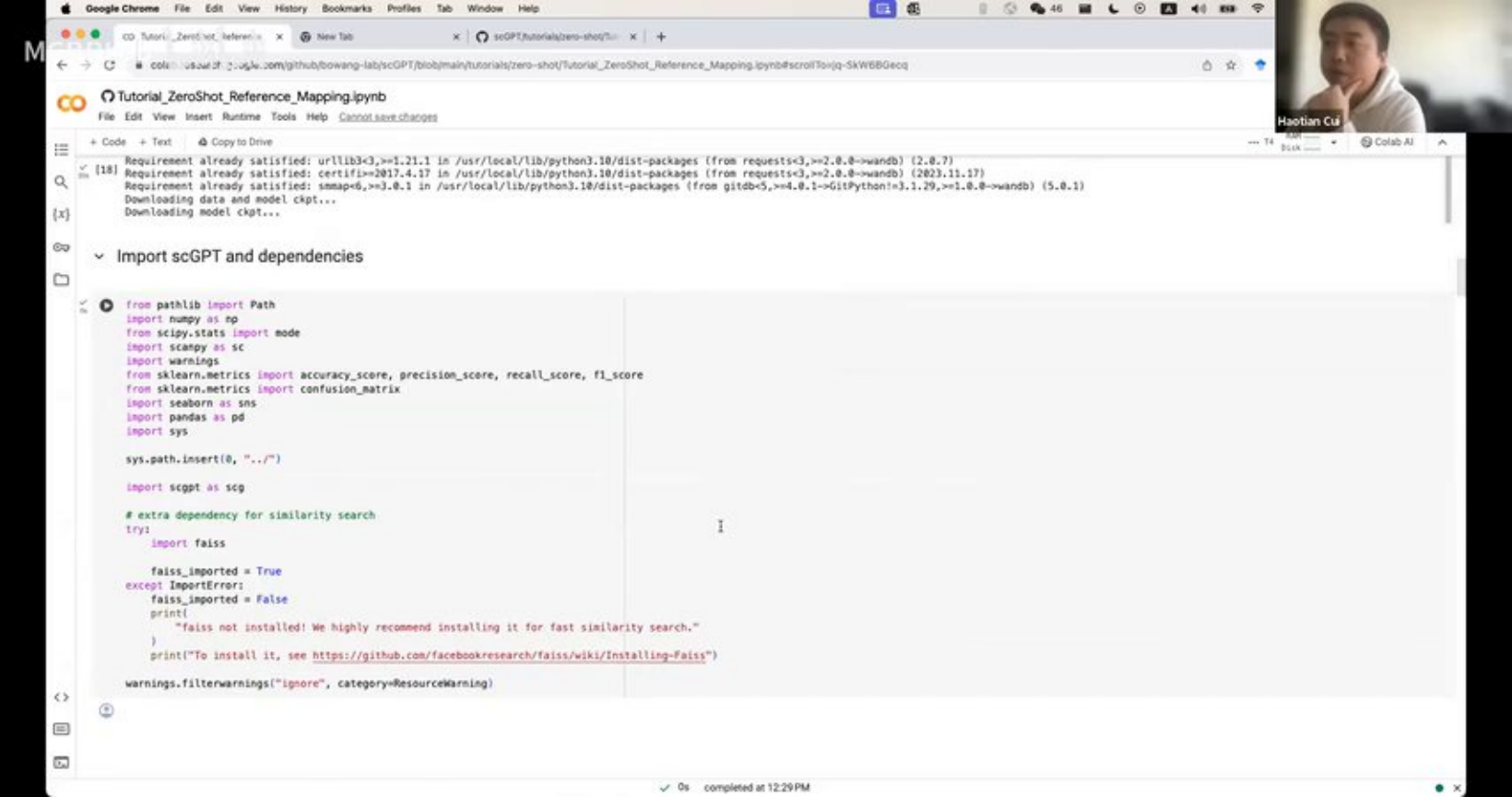
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[18] Requirement already satisfied: urllib3<3,>=1.21.1 in /usr/local/lib/python3.10/dist-packages (from requests<3,>=2.0.0->wandb) (2.0.7)
Requirement already satisfied: certifi>=2017.4.17 in /usr/local/lib/python3.10/dist-packages (from requests<3,>=2.0.0->wandb) (2023.11.17)
Requirement already satisfied: smmap<6,>=3.0.1 in /usr/local/lib/python3.10/dist-packages (from gitdb<5,>=4.0.1->GitPython!=3.1.29,>=1.0.0->wandb) (5.0.1)
Downloading data and model ckpt...
Downloading model ckpt...
Import scGPT and dependencies
from pathlib import Path
import numpy as np
from scipy.stats import mode
import scanpy as sc
import warnings
from sklearn.metrics import accuracy_score, precision_score, recall_score, f1_score
from sklearn.metrics import confusion_matrix
import seaborn as sns
import pandas as pd
import sys
sys.path.insert(0, "../")
import scgpt as scg
# extra dependency for similarity search
try:
import faiss
faiss_imported = True
except ImportError:
faiss_imported = False
print(
"faiss not installed! We highly recommend installing it for fast similarity search."
)
print("To install it, see https://github.com/facebookresearch/faiss/wiki/Installing-Faiss")
warnings.filterwarnings("ignore", category=ResourceWarning)
0s completed at 12:29 PM

Tutorial_ZeroShot_Reference_Mapping.ipynb

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[19]

Load the dataset, you may download the dataset from here. We set the columns storing gene name columns, batch key and cell type key.

```
model_dir = Path("../../save/scGPT_human")
adata = sc.read_h5ad('../../data/covid/batch_covid_subsampled_train.h5ad')
test_adata = sc.read_h5ad('../../data/covid/batch_covid_subsampled_test.h5ad')

cell_type_key = "celltype"
gene_col = "gene_name"
```

```
/usr/local/lib/python3.10/dist-packages/ipykernel/ipkernel.py:283: DeprecationWarning: `should_run_async` will not call `transform_cell` automatically in the future. Please pass the result to `transformed_cell` ar
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```

Embed the reference dataset

```
ref_embed_adata = scg.tasks.embed_data(
    adata,
    model_dir,
    gene_col=gene_col,
    batch_size=64,
)
```

```
scGPT - INFO - match 1173/1200 genes in vocabulary of size 60697.
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  warnings.warn(
Embedding cells:  94%|[redacted]| 236/250 [00:32<00:01,  7.38it/s]
```

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Embed the reference dataset

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  adata.obsm["X_scGPT"] = cell_embeddings
```

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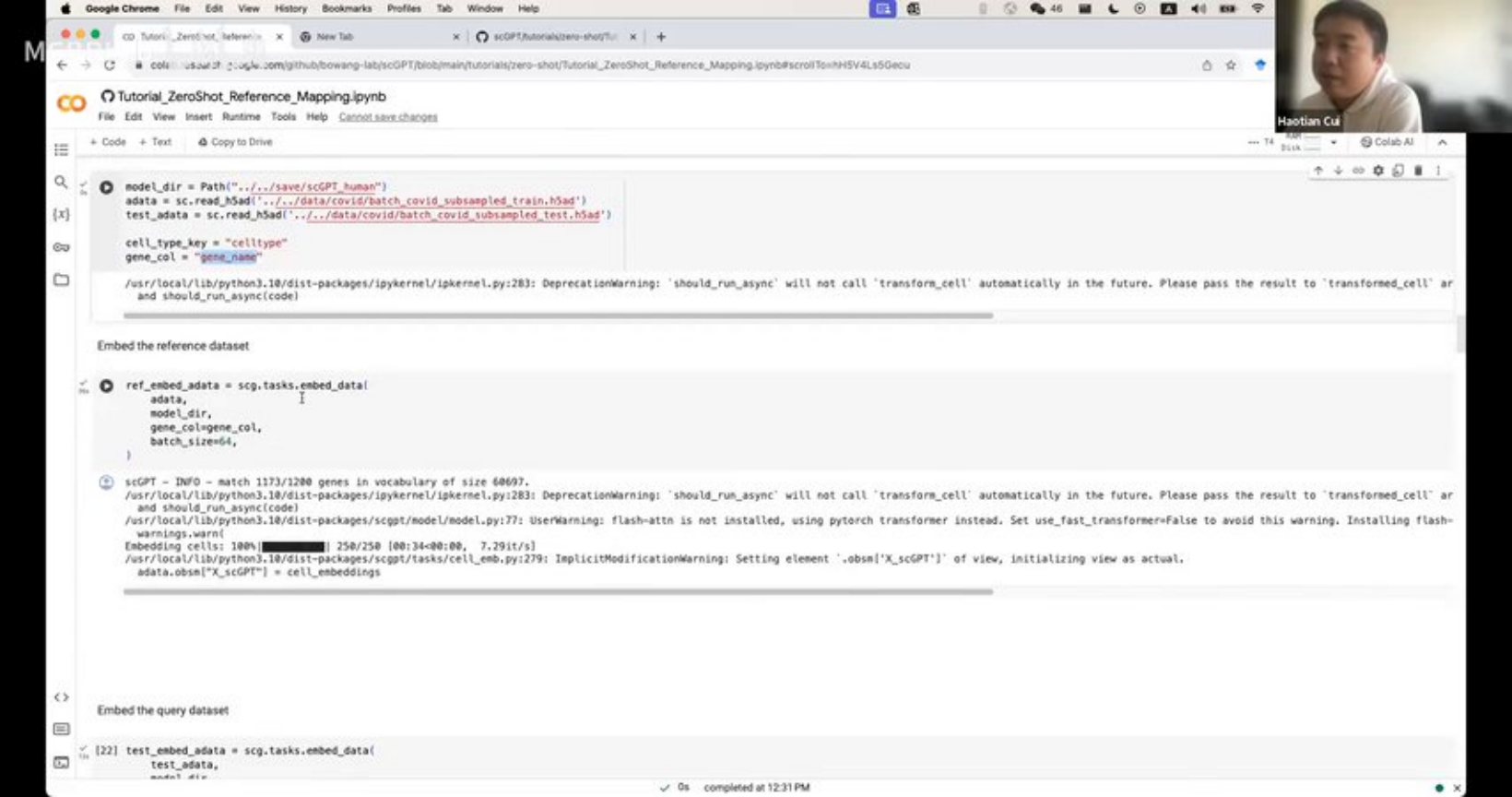
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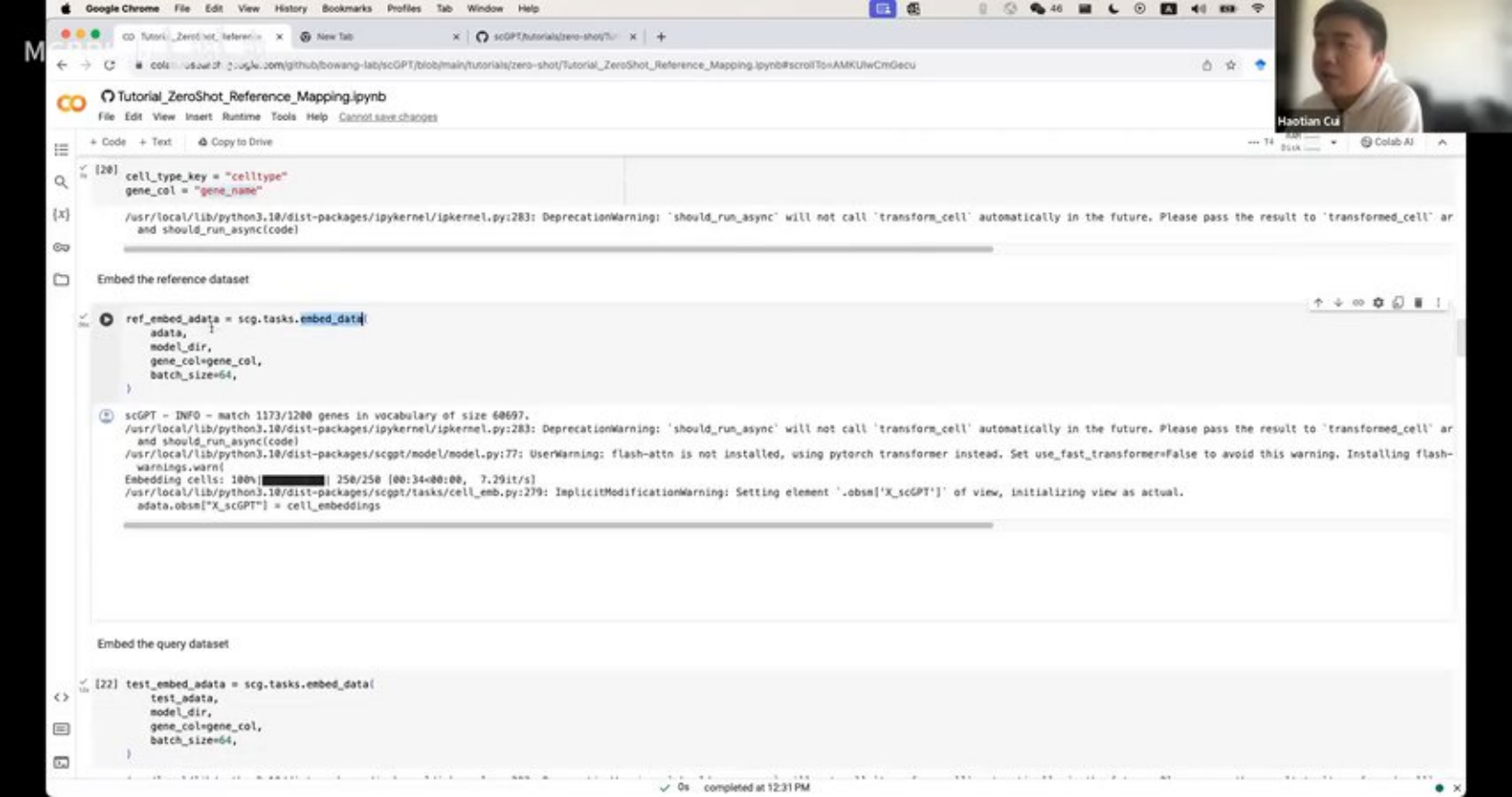
Embed the query dataset
[22] test_embed_adata = scg.tasks.embed_data(
test_adata,
0s completed at 12:31 PM
Haotian Cui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Tutorial_ZeroShot_Reference_Mapping.ipynb
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[20] cell_type_key = "celltype"
gene_col = "gene_name"
/usr/local/lib/python3.10/dist-packages/ipykernel/ipkernel.py:283: DeprecationWarning: `should_run_async` will not call `transform_cell` automatically in the future. Please pass the result to `transformed_cell` ar
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0s completed at 12:31 PM

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Embedding cells: 100%|██████████| 63/63 [00:09<00:00,  6.86it/s]
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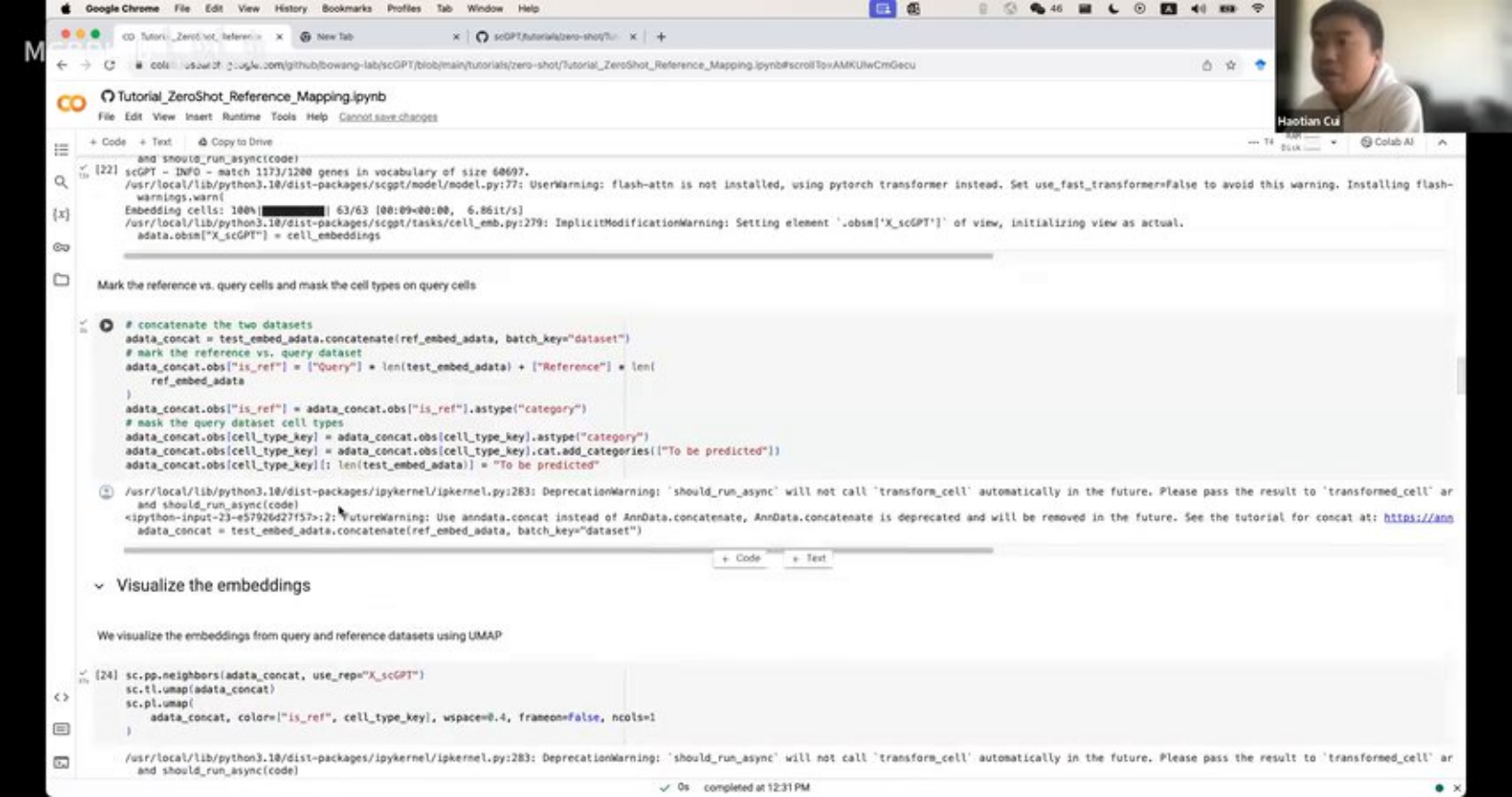
  adata.obsm["X_scGPT"] = cell_embeddings
```

Mark the reference vs. query cells and mask the cell types on query cells

```
[23] # concatenate the two datasets
     adata_concat = test_embed_adata.concatenate(ref_embed_adata, batch_key="dataset")
     # mark the reference vs. query dataset
```

0s completed at 12:31 PM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adata_concat = test_embed_adata.concatenate(ref_embed_adata, batch_key="dataset")
# mark the reference vs. query dataset
adata_concat.obs["is_ref"] = ["Query"] * len(test_embed_adata) + ["Reference"] * len(
ref_embed_adata
)
adata_concat.obs["is_ref"] = adata_concat.obs["is_ref"].astype("category")
# mask the query dataset cell types
adata_concat.obs[cell_type_key] = adata_concat.obs[cell_type_key].astype("category")
adata_concat.obs[cell_type_key] = adata_concat.obs[cell_type_key].cat.add_categories(["To be predicted"])
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+ Code + Text
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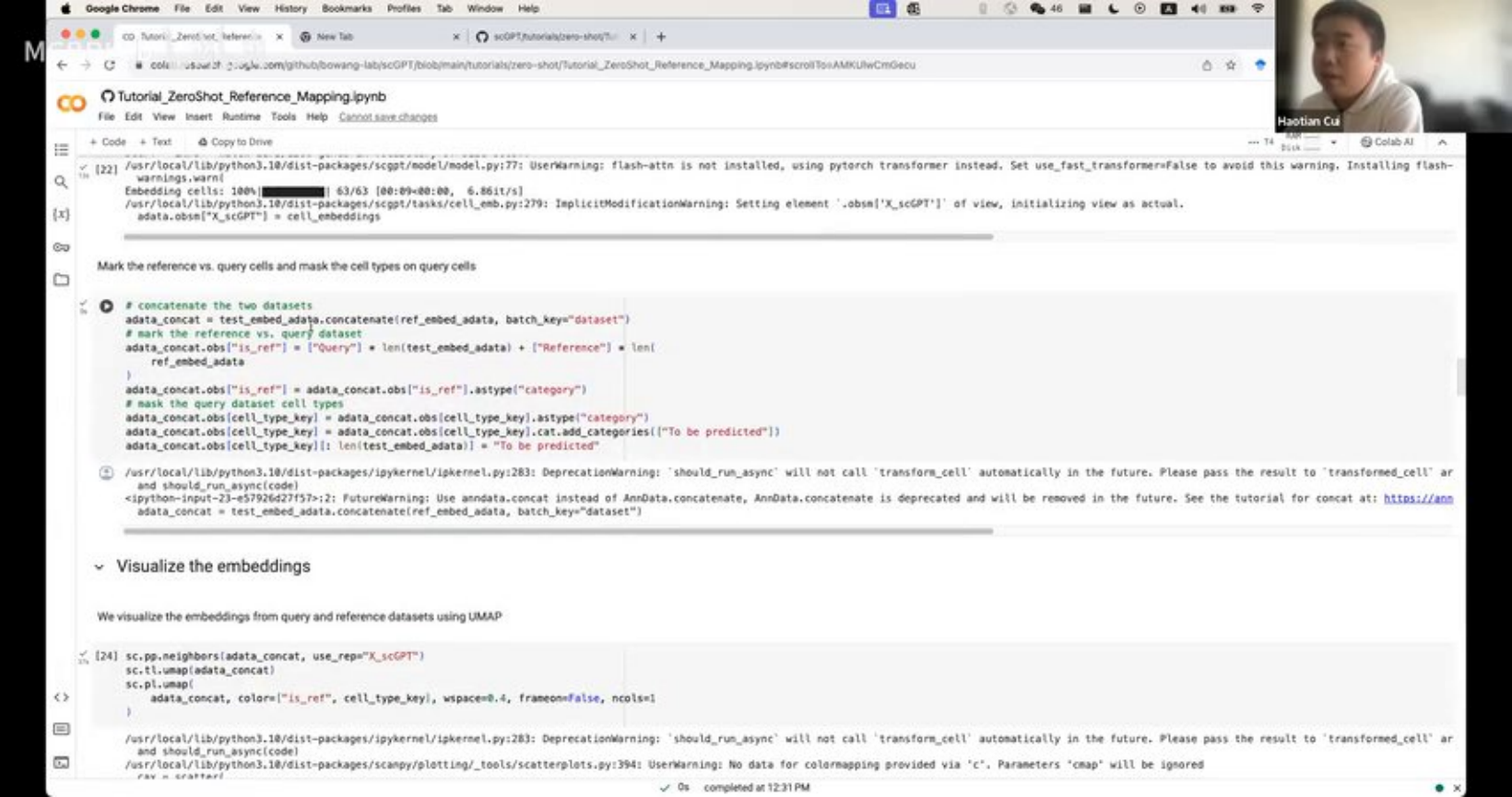
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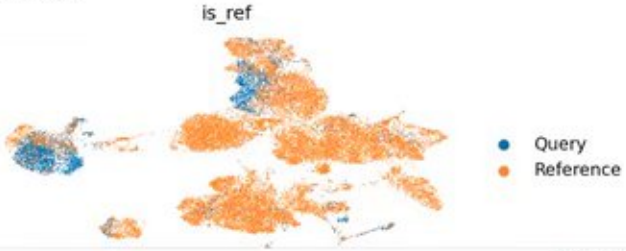

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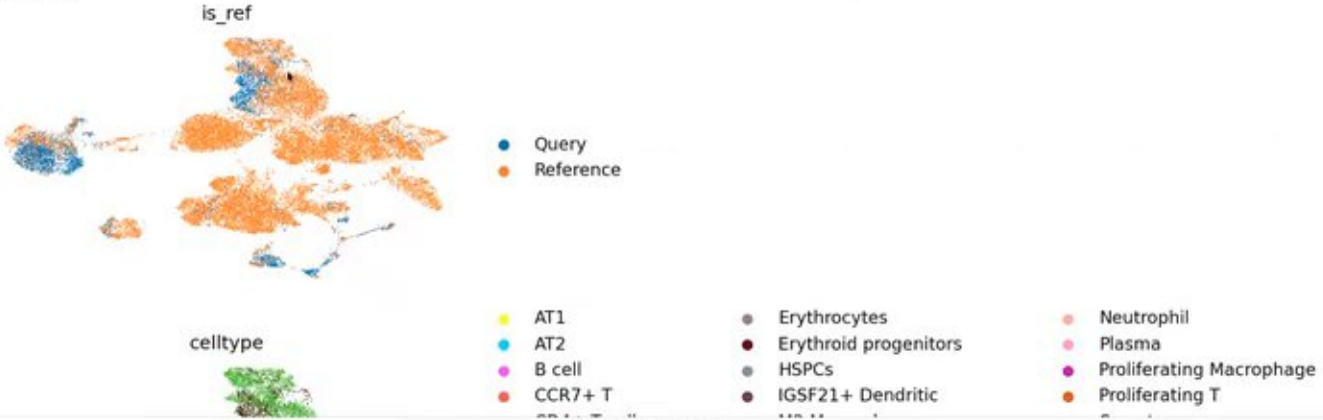

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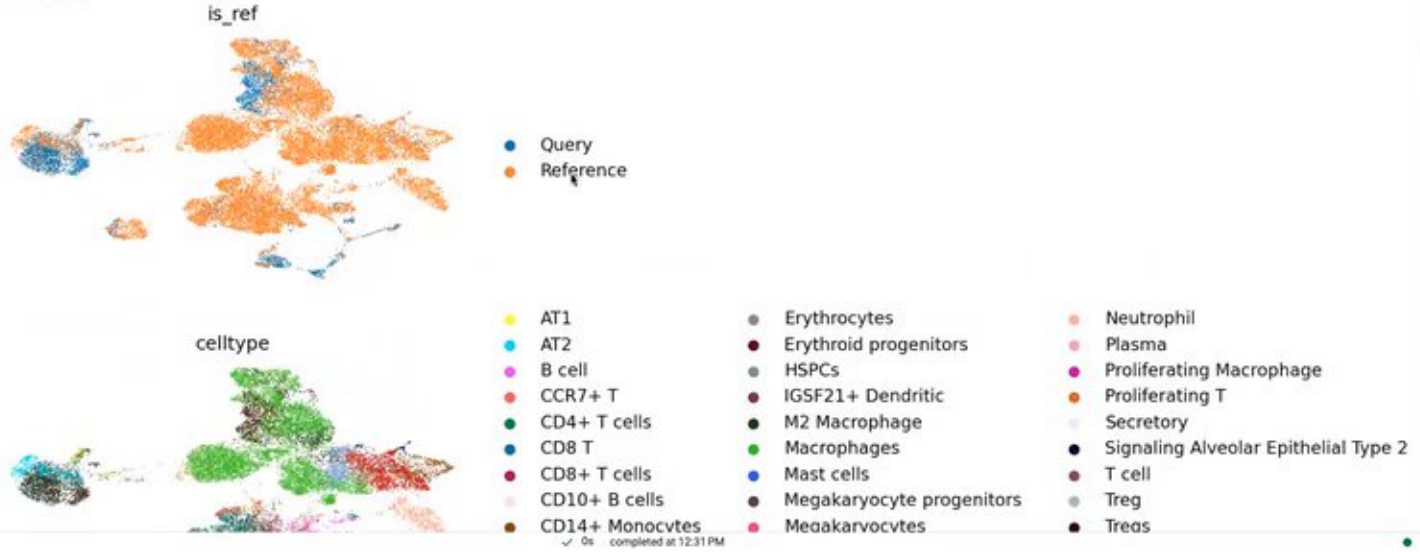

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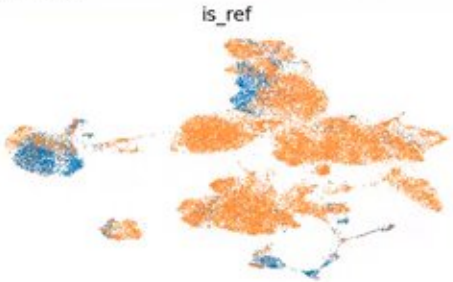
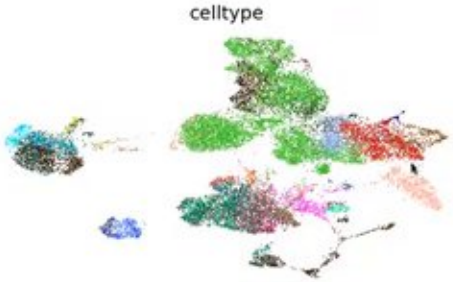
```
    cax = scatter(
/usr/local/lib/python3.10/dist-packages/scanpy/plotting/_tools/scatterplots.py:394: UserWarning: No data for colormapping provided via 'c'. Parameters 'cmap' will be ignored
    cax = scatter(
```



- Query
- Reference



- AT1
- AT2
- B cell
- CCR7+ T
- CD4+ T cells
- CD8 T
- CD8+ T cells
- CD10+ B cells
- CD14+ Monocytes
- CD16+ Monocytes
- CD20+ B cells
- Ciliated
- DC_activated
- Erythrocytes
- Erythroid progenitors
- HSPCs
- IGSF21+ Dendritic
- M2 Macrophage
- Macrophages
- Mast cells
- Megakaryocyte progenitors
- Megakaryocytes
- Monocyte progenitors
- Monocytes
- NK
- NKT cells
- Neutrophil
- Plasma
- Proliferating Macrophage
- Proliferating T
- Secretory
- Signaling Alveolar Epithelial Type 2
- T cell
- Treg
- Tregs
- innate T
- mDC
- pDC
- To be predicted

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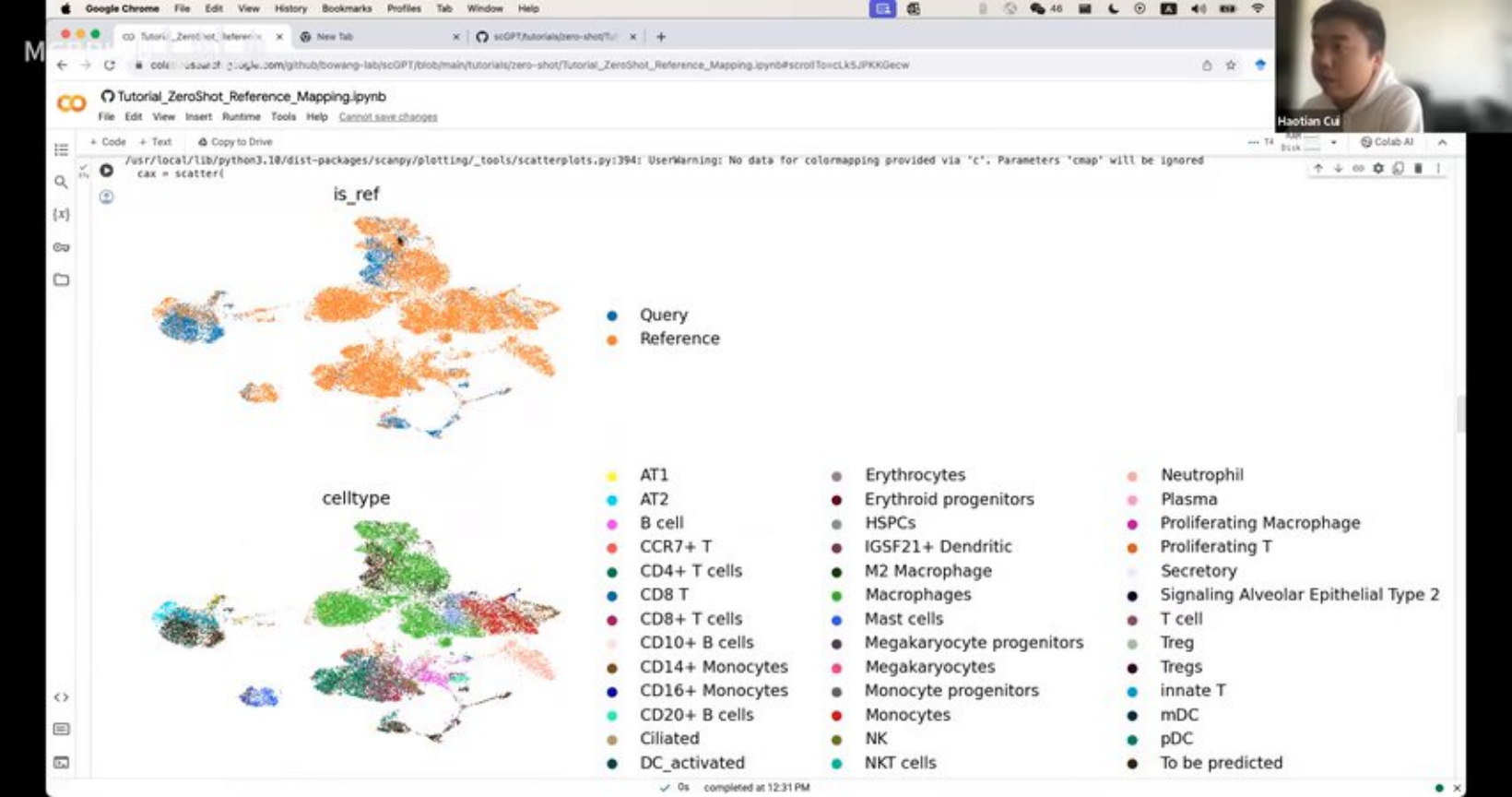
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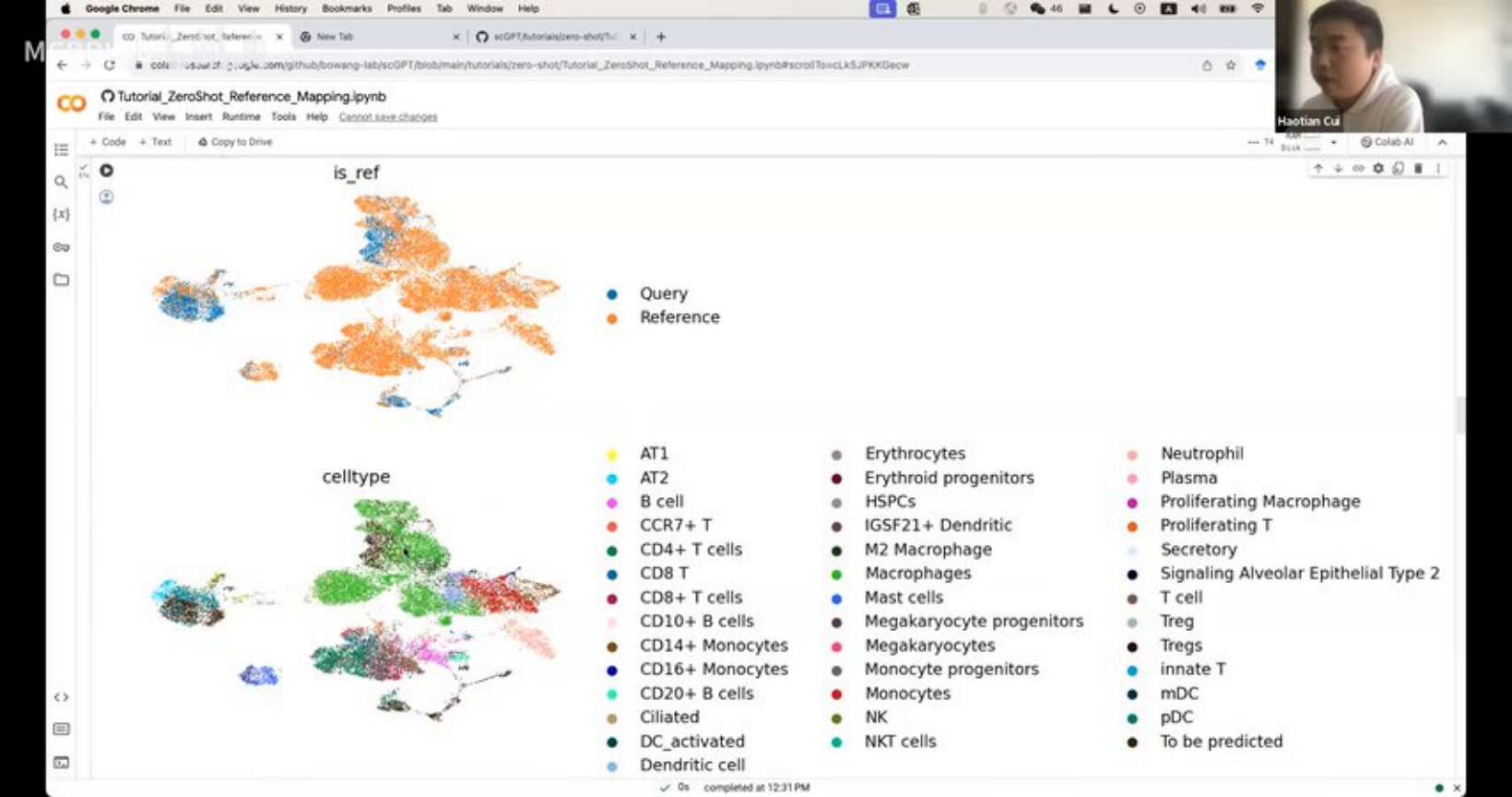
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Query
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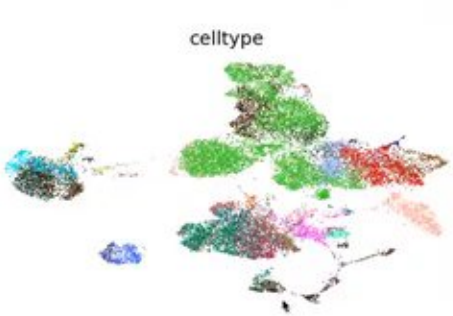
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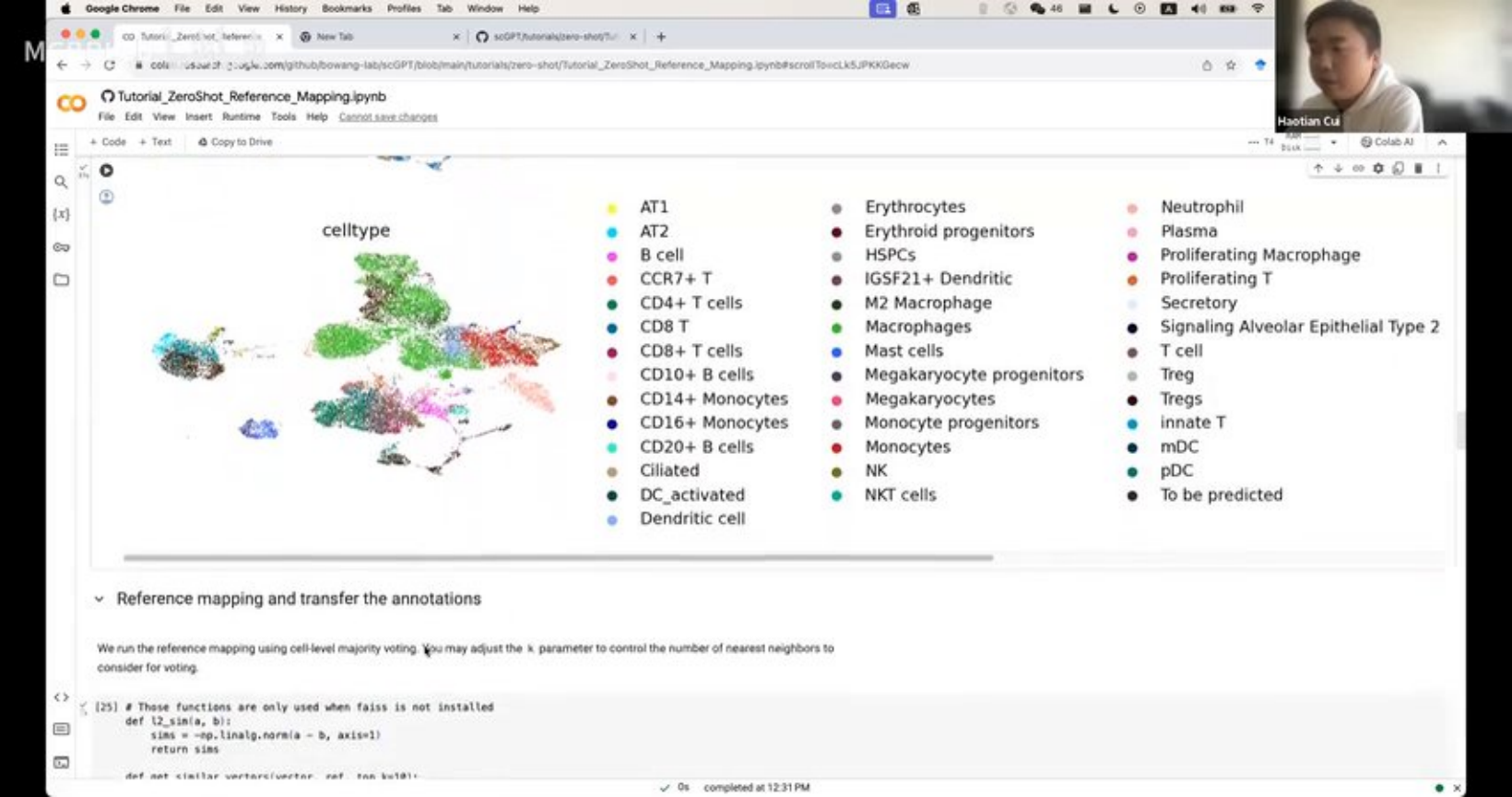
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To be predicted
Reference mapping and transfer the annotations
We run the reference mapping using cell-level majority voting. You may adjust the k parameter to control the number of nearest neighbors to consider for voting.
[25] # Those functions are only used when faiss is not installed
def l2_sim(a, b):
sims = -np.linalg.norm(a - b, axis=1)
return sims
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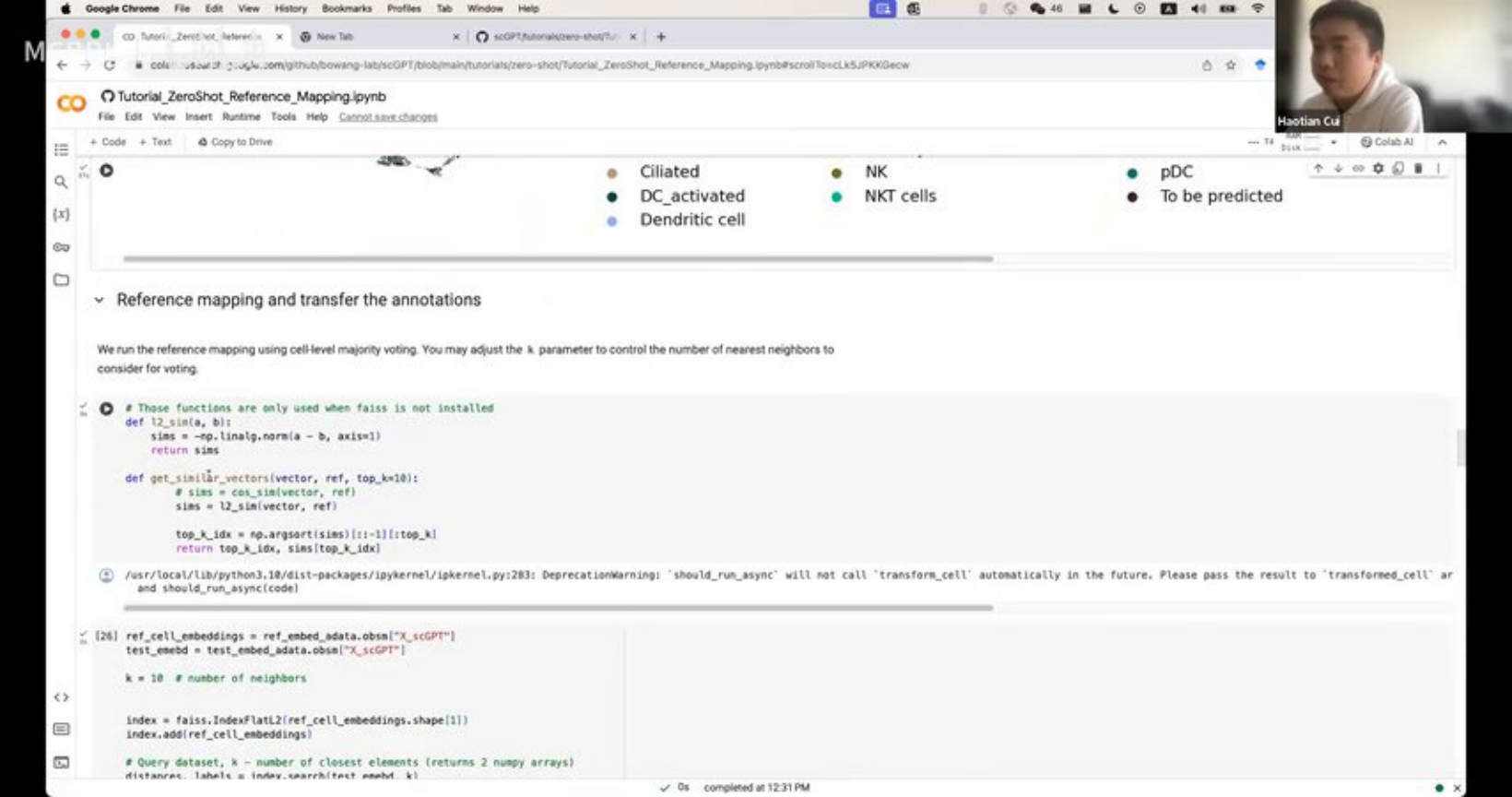
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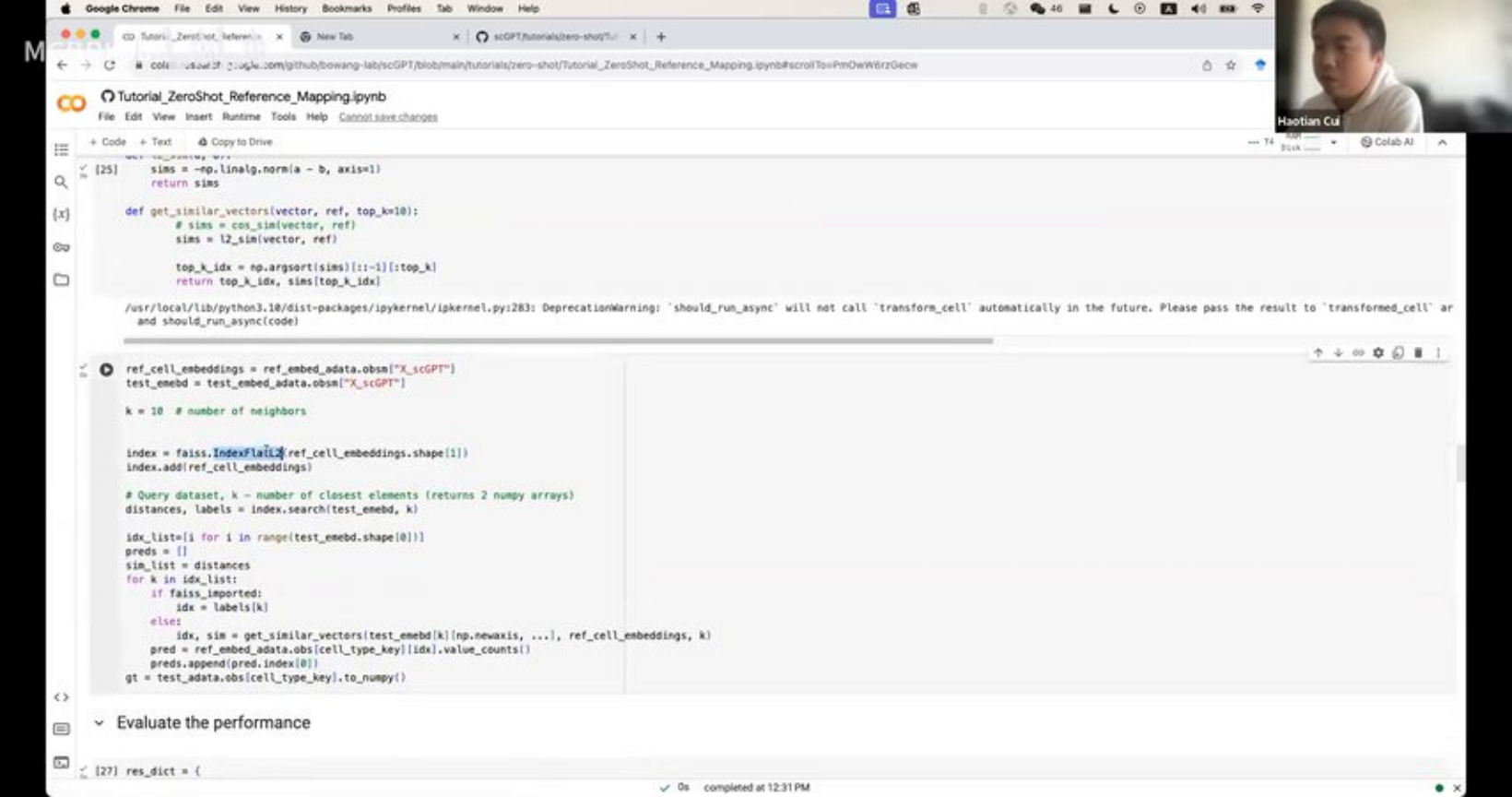
def l2_sim(a, b):
sims = -np.linalg.norm(a - b, axis=1)
return sims
def get_similar_vectors(vector, ref, top_k=10):
# sims = cos_sim(vector, ref)
sims = l2_sim(vector, ref)
top_k_idx = np.argsort(sims)[::-1][:top_k]
return top_k_idx, sims[top_k_idx]
/usr/local/lib/python3.10/dist-packages/ipykernel/ipkernel.py:283: DeprecationWarning: `should_run_async` will not call `transform_cell` automatically in the future. Please pass the result to `transformed_cell` ar
and should_run_async(code)
[26] ref_cell_embeddings = ref_embed_adata.obsm["X_scGPT"]
test_emebd = test_embed_adata.obsm["X_scGPT"]
k = 10 # number of neighbors
index = faiss.IndexFlatL2(ref_cell_embeddings.shape[1])
index.add(ref_cell_embeddings)
# Query dataset, k - number of closest elements (returns 2 numpy arrays)
0s completed at 12:31 PM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# Query dataset, k - number of closest elements (returns 2 numpy arrays)
distances, labels = index.search(test_emebd, k)
idx_list=[i for i in range(test_emebd.shape[0])]
preds = []
sim_list = distances
for k in idx_list:
if faiss_imported:
idx = labels[k]
else:
idx, sim = get_similar_vectors(test_emebd[k][np.newaxis, ...], ref_cell_embeddings, k)
pred = ref_embed_adata.obs[cell_type_key][idx].value_counts()
preds.append(pred.index[0])
gt = test_adata.obs[cell_type_key].to_numpy()
Evaluate the performance
[27] res_dict = {
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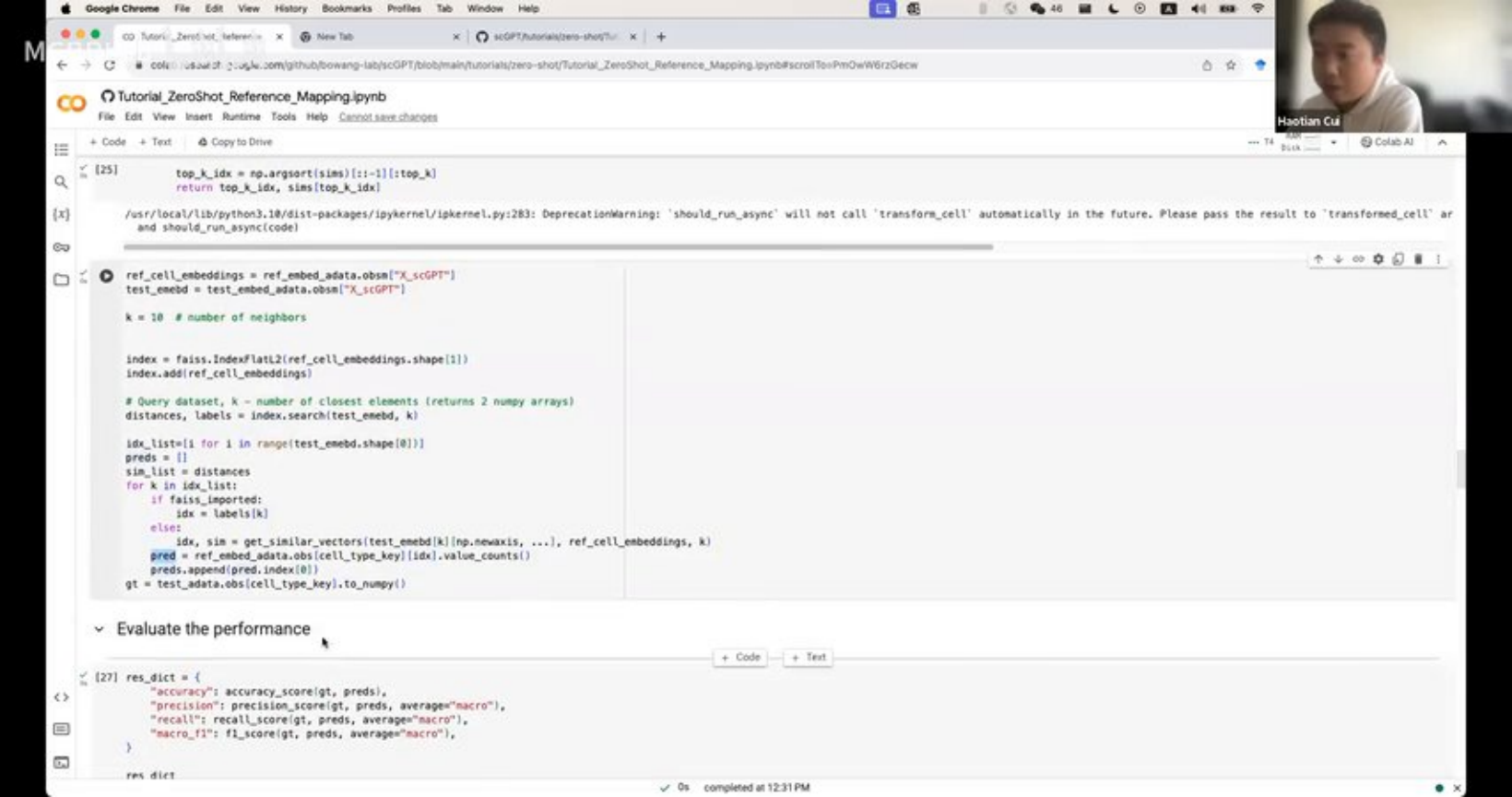

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[25]
```
        top_k_idx = np.argsort(sims)[::-1][:top_k]
        return top_k_idx, sims[top_k_idx]
```

```
/usr/local/lib/python3.10/dist-packages/ipykernel/ipkernel.py:283: DeprecationWarning: `should_run_async` will not call `transform_cell` automatically in the future. Please pass the result to `transformed_cell` ar
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    else:
        idx, sim = get_similar_vectors(test_emebd[k][np.newaxis, ...], ref_cell_embeddings, k)
    pred = ref_embed_adata.obs[cell_type_key][idx].value_counts()
    preds.append(pred.index[0])
gt = test_adata.obs[cell_type_key].to_numpy()
```

Evaluate the performance

+ Code + Text

[27]
```
res_dict = {
    "accuracy": accuracy_score(gt, preds),
    "precision": precision_score(gt, preds, average="macro"),
    "recall": recall_score(gt, preds, average="macro"),
    "macro_f1": f1_score(gt, preds, average="macro"),
}

res_dict
```

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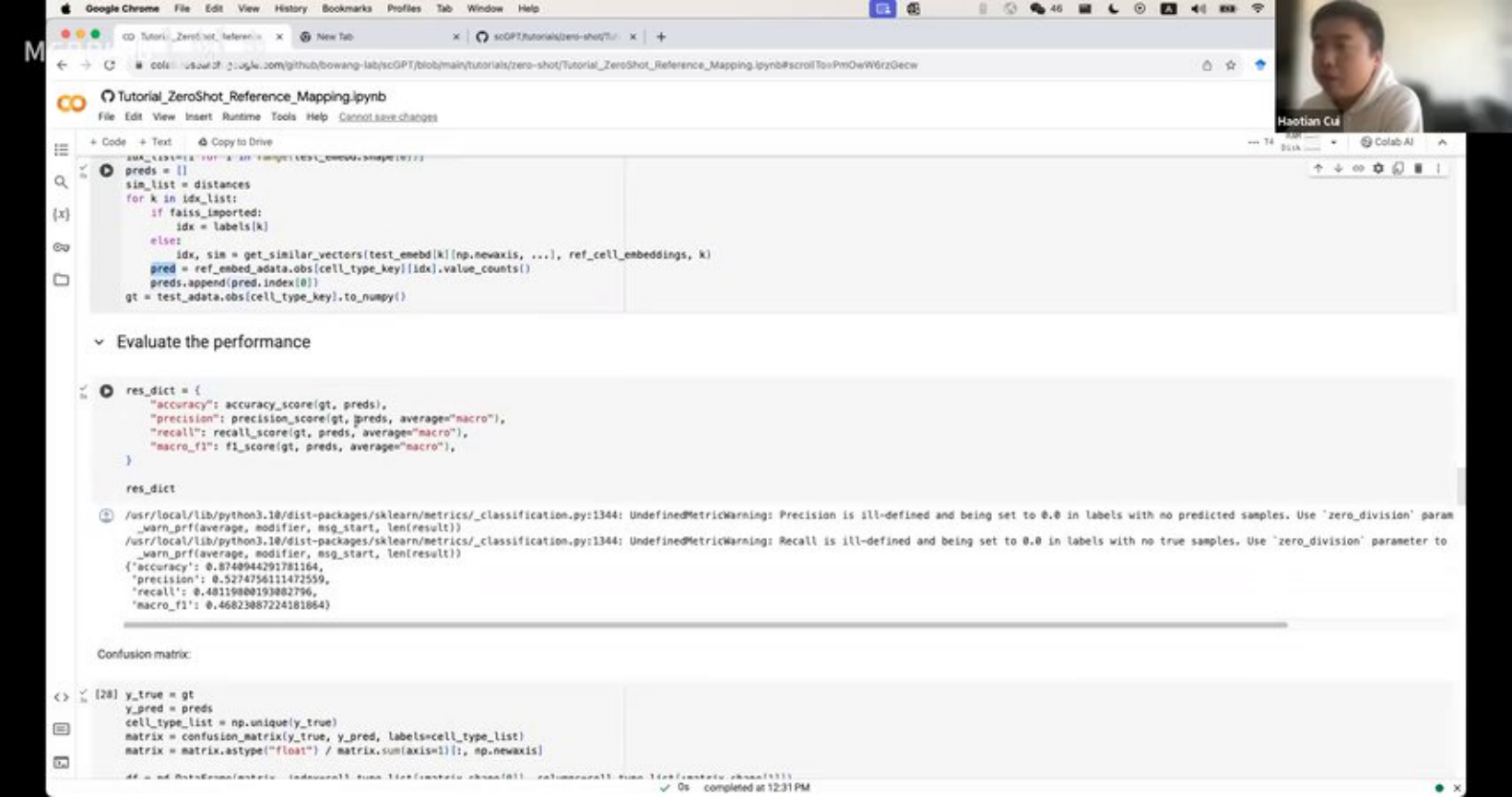
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Colab AI
Haotian Cui
preds = []
sim_list = distances
for k in idx_list:
if faiss_imported:
idx = labels[k]
else:
idx, sim = get_similar_vectors(test_emebd[k][np.newaxis, ...], ref_cell_embeddings, k)
pred = ref_embed_adata.obs[cell_type_key][idx].value_counts()
preds.append(pred.index[0])
gt = test_adata.obs[cell_type_key].to_numpy()
Evaluate the performance
res_dict = {
"accuracy": accuracy_score(gt, preds),
"precision": precision_score(gt, preds, average="macro"),
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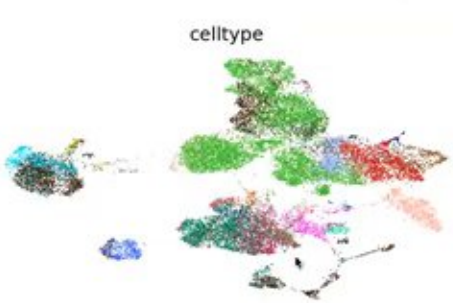
}
res_dict
/usr/local/lib/python3.10/dist-packages/sklearn/metrics/_classification.py:1344: UndefinedMetricWarning: Precision is ill-defined and being set to 0.0 in labels with no predicted samples. Use `zero_division` param
_warn_prf(average, modifier, msg_start, len(result))
/usr/local/lib/python3.10/dist-packages/sklearn/metrics/_classification.py:1344: UndefinedMetricWarning: Recall is ill-defined and being set to 0.0 in labels with no true samples. Use `zero_division` parameter to
_warn_prf(average, modifier, msg_start, len(result))
{'accuracy': 0.8740944291781164,
'precision': 0.5274756111472559,
'recall': 0.4811980019302796,
'macro_f1': 0.4682308722418186}
Confusion matrix:
[28] y_true = gt
y_pred = preds
cell_type_list = np.unique(y_true)
matrix = confusion_matrix(y_true, y_pred, labels=cell_type_list)
matrix = matrix.astype("float") / matrix.sum(axis=1)[:, np.newaxis]
0s completed at 12:31 PM


Query
Reference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```
distances, labels = index.search(test_emebd, k)

idx_list=[i for i in range(test_emebd.shape[0])]
preds = []
sim_list = distances
for k in idx_list:
    if faiss_imported:
        idx = labels[k]
    else:
        idx, sim = get_similar_vectors(test_emebd[k][np.newaxis, ...], ref_cell_embeddings, k)
    pred = ref_embed_adata.obs[cell_type_key][idx].value_counts()
    preds.append(pred.index[0])
gt = test_adata.obs[cell_type_key].to_numpy()
```

Evaluate the performance

```
res_dict = {
    "accuracy": accuracy_score(gt, preds),
    "precision": precision_score(gt, preds, average="macro"),
    "recall": recall_score(gt, preds, average="macro"),
    "macro_f1": f1_score(gt, preds, average="macro"),
}

res_dict
```

```
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 'precision': 0.5274756111472559,
 'recall': 0.4811980019308279,
 'macro_f1': 0.4682308722418106}
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Confusion matrix:

```
[28] y_true = gt
     y_pred = preds
     cell_type_list = np.unique(y_true)
     matrix = confusion_matrix(y_true, y_pred, labels=cell_type_list)
```

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```
        else:
            idx, sim = get_similar_vectors(test_emebd[k][np.newaxis, ...], ref_cell_embeddings, k)
        pred = ref_embed_adata.obs[cell_type_key][idx].value_counts()
        preds.append(pred.index[0])
    gt = test_adata.obs[cell_type_key].to_numpy()
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Evaluate the performance

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     matrix = matrix.astype("float") / matrix.sum(axis=1)[:, np.newaxis]

     df = pd.DataFrame(matrix, index=cell_type_list[:matrix.shape[0]], columns=cell_type_list[:matrix.shape[1]])

     ax = sns.clustermap(df,
                         cmap='Purples',
                         annot=True ,fmt=".2f",
                         annot_kws={'size': 8},
```

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Evaluate the performance

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[27] res_dict = {
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    res_dict
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ax = sns.clustermap(df,
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                    annot=True ,fmt=".2f",
                    annot_kws={'size': 8},
                    vmin=0,
                    vmax=1,
                    row_cluster=False,
                    col_cluster=False,
                    figsize=(14, 14))
```

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y_true = gt
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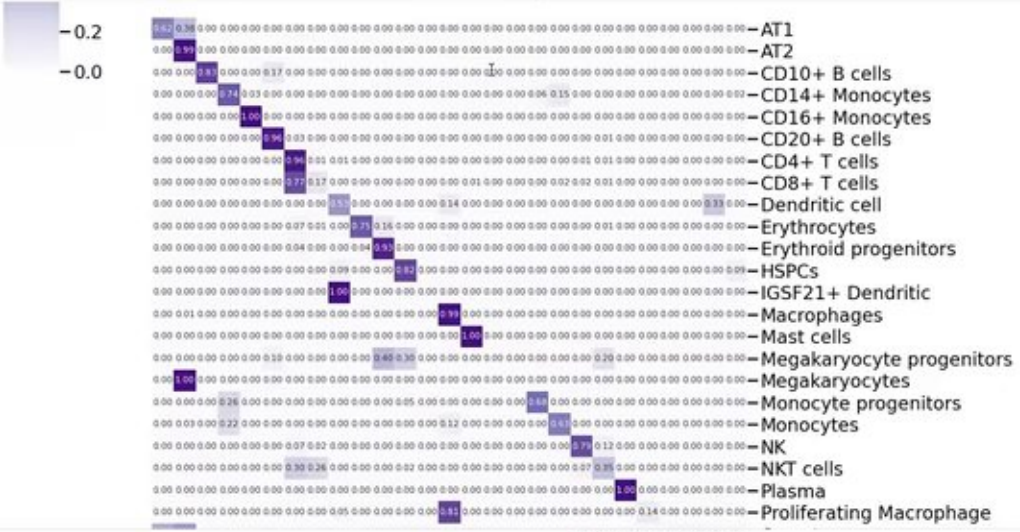
                    figsize=(14, 14))
```



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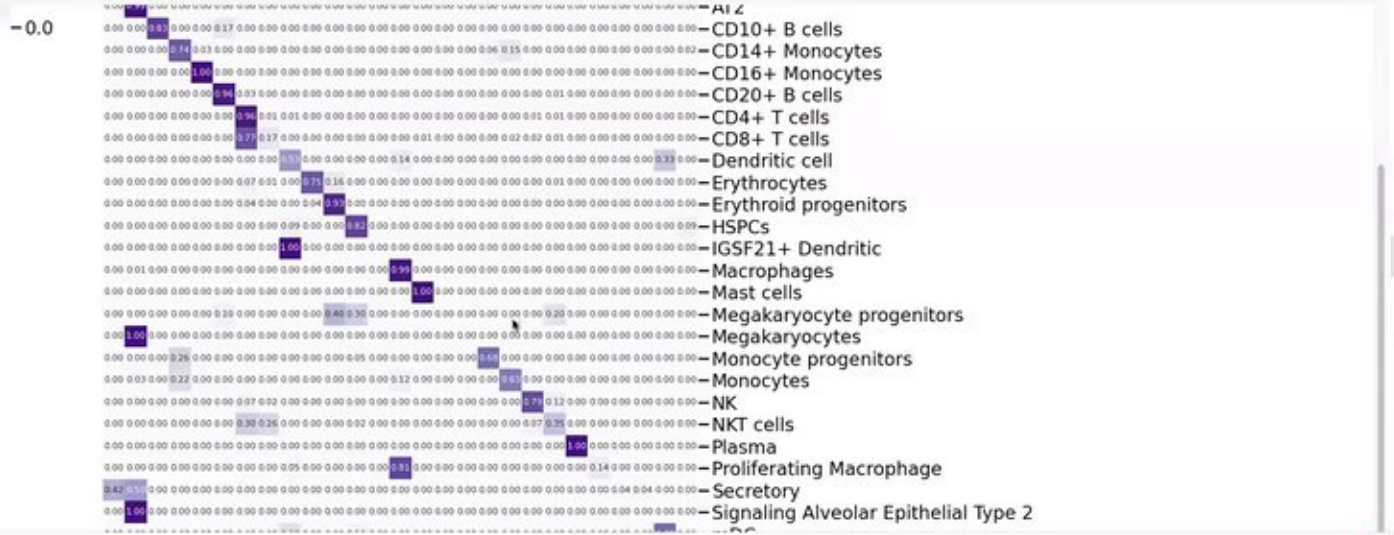
```
ax = sns.clustermap(df,
                    cmap='Purples',
                    annot=True ,fmt=".2f",
                    annot_kws={'size': 8},
                    vmin=0,
                    vmax=1,
                    row_cluster=False,
                    col_cluster=False,
                    figsize=(14, 14))
```



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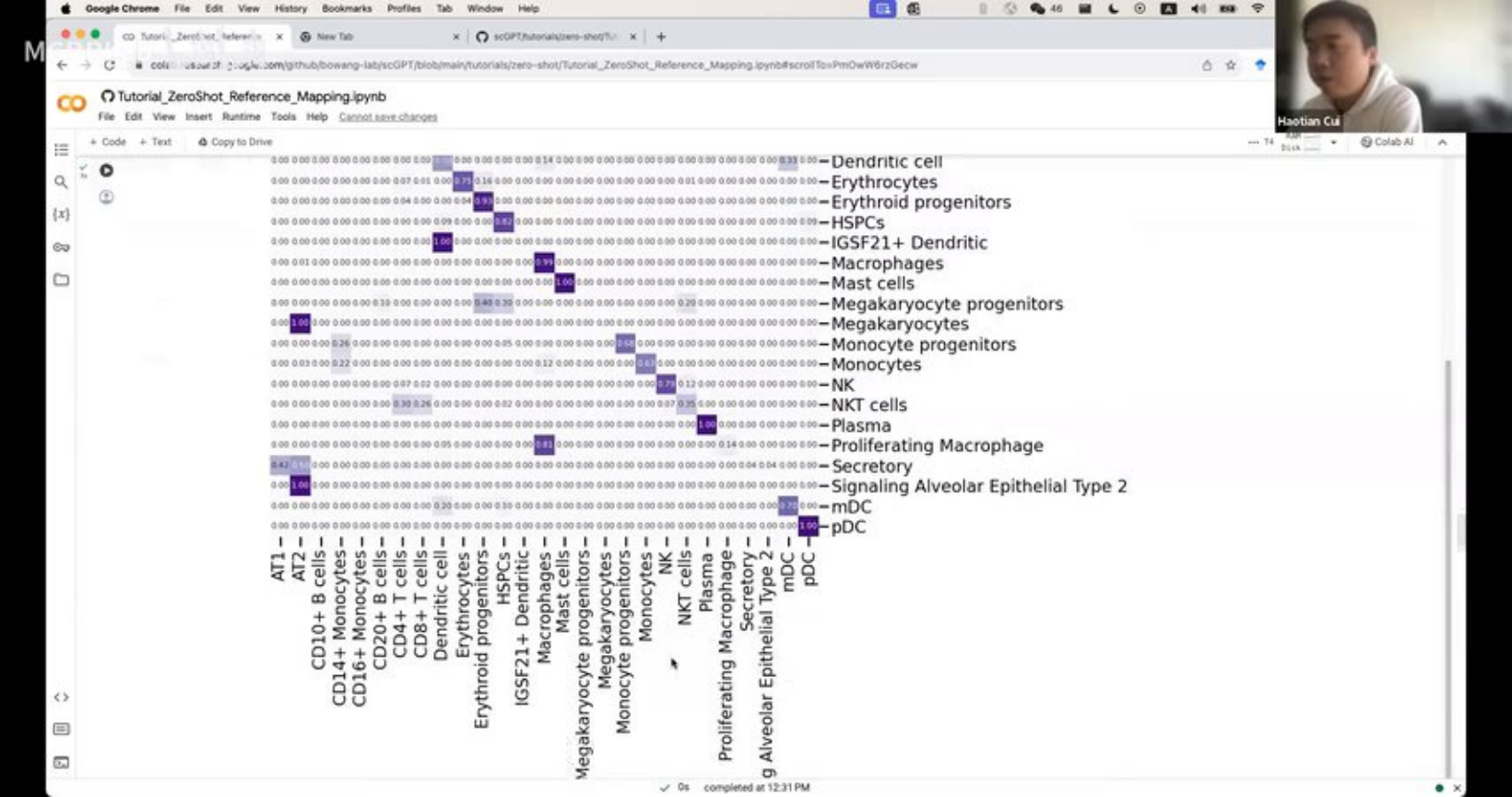
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Dendritic cell
Erythrocytes
Erythroid progenitors
HSPCs
IGSF21+ Dendritic
Macrophages
Mast cells
Megakaryocyte progenitors
Megakaryocytes
Monocyte progenitors
Monocytes
NK
NKT cells
Plasma
Proliferating Macrophage
Secretory
Signaling Alveolar Epithelial Type 2
mDC
pDC
AT1
AT2
CD10+ B cells
CD14+ Monocytes
CD16+ Monocytes
CD20+ B cells
CD4+ T cells
CD8+ T cells
Dendritic cell
Erythrocytes
Erythroid progenitors
HSPCs
IGSF21+ Dendritic
Macrophages
Mast cells
Megakaryocyte progenitors
Megakaryocytes
Monocyte progenitors
Monocytes
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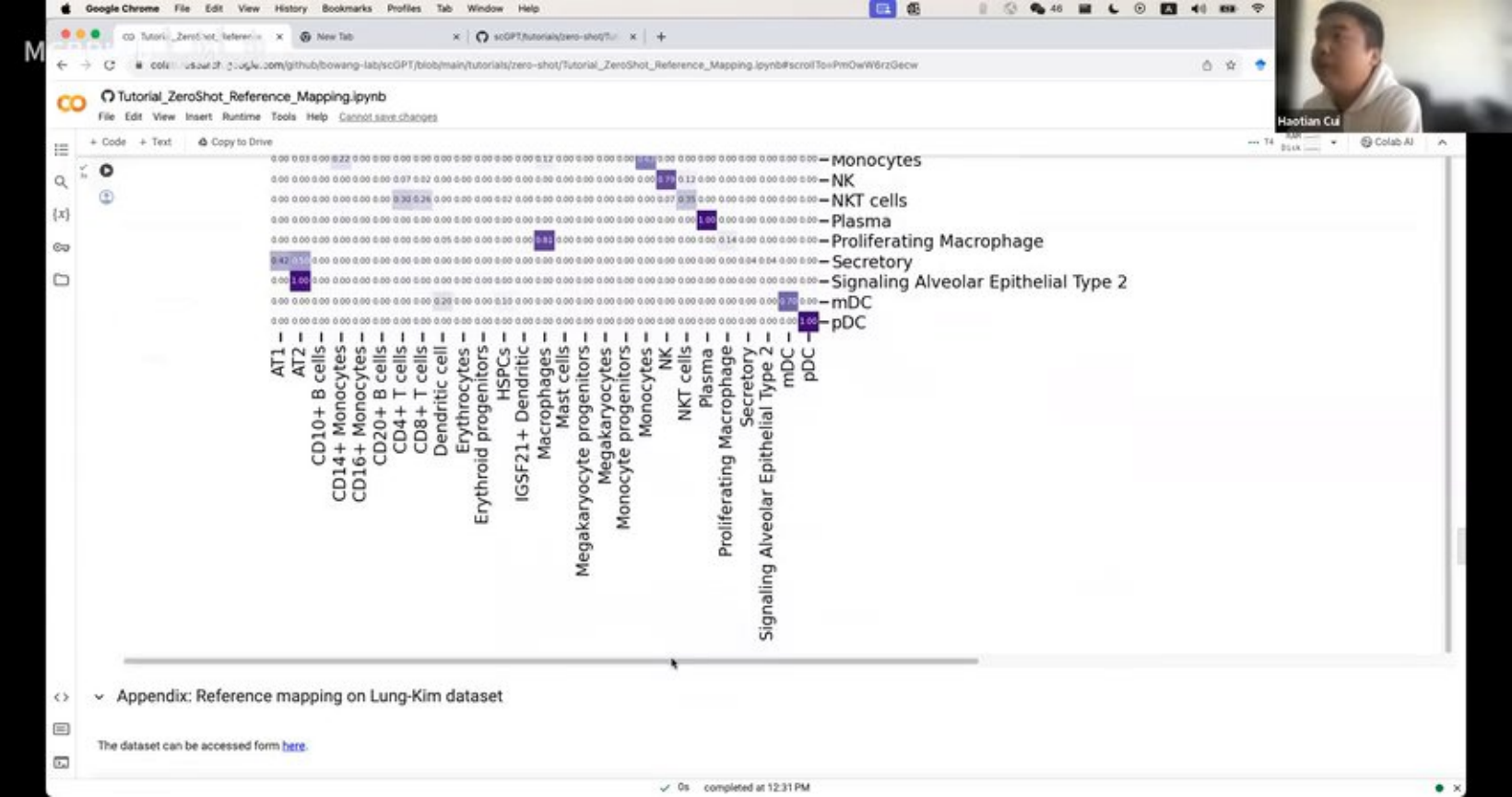
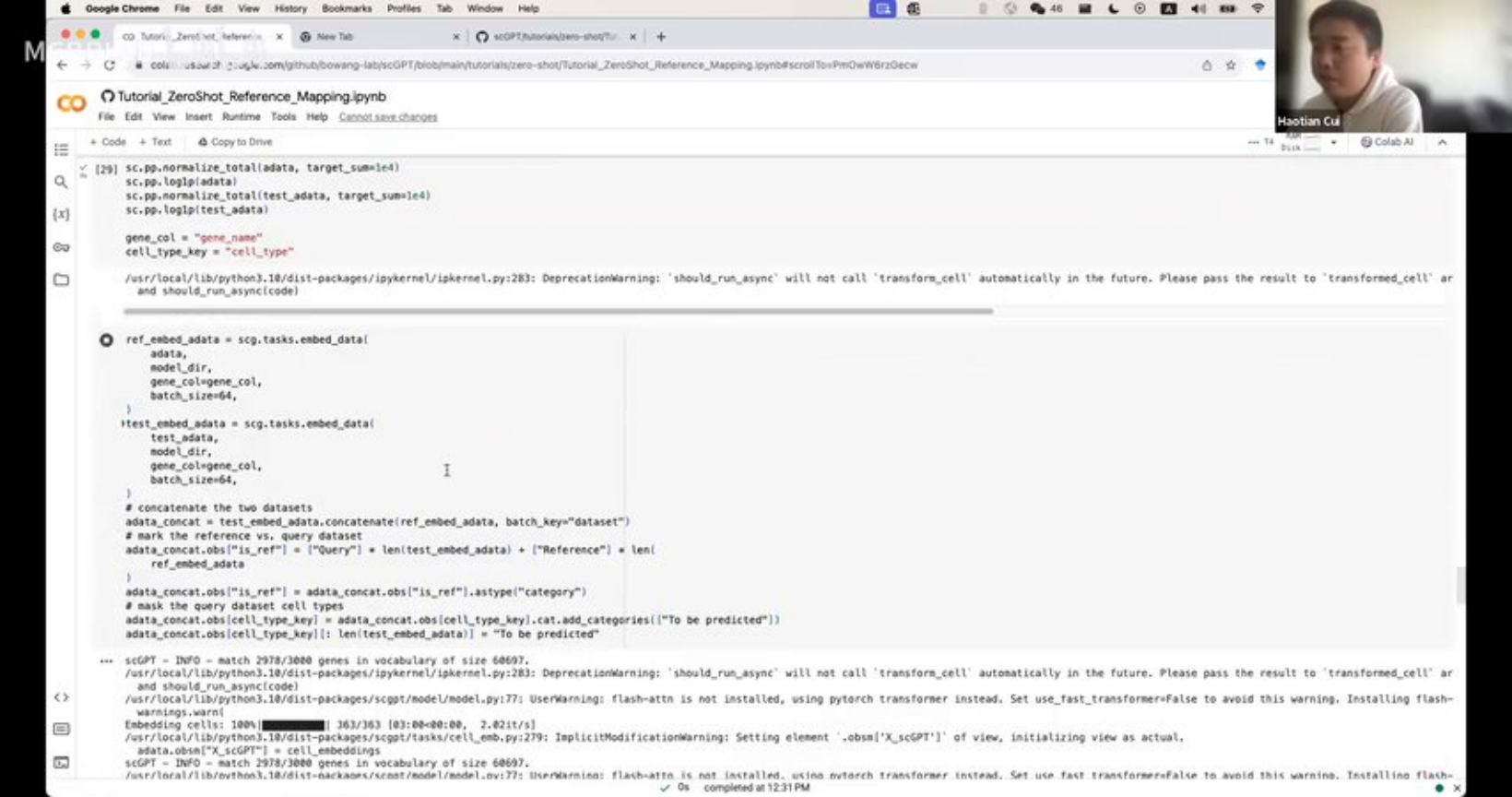


Appendix: Reference mapping on Lung-Kim dataset

The dataset can be accessed form here.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[29] sc.pp.normalize_total(adata, target_sum=1e4)
sc.pp.log1p(adata)
sc.pp.normalize_total(test_adata, target_sum=1e4)
sc.pp.log1p(test_adata)
gene_col = "gene_name"
cell_type_key = "cell_type"
/usr/local/lib/python3.10/dist-packages/ipykernel/ipkernel.py:283: DeprecationWarning: 'should_run_async' will not call 'transform_cell' automatically in the future. Please pass the result to 'transformed_cell' ar
and should_run_async(code)
ref_embed_adata = scg.tasks.embed_data(
adata,
model_dir,
gene_col=gene_col,
batch_size=64,
)
test_embed_adata = scg.tasks.embed_data(
test_adata,
model_dir,
gene_col=gene_col,
batch_size=64,
)
# concatenate the two datasets
adata_concat = test_embed_adata.concatenate(ref_embed_adata, batch_key="dataset")
# mark the reference vs. query dataset
adata_concat.obs["is_ref"] = ["Query"] * len(test_embed_adata) + ["Reference"] * len(
ref_embed_adata
)
adata_concat.obs["is_ref"] = adata_concat.obs["is_ref"].astype("category")
# mask the query dataset cell types
adata_concat.obs[cell_type_key] = adata_concat.obs[cell_type_key].cat.add_categories(["To be predicted"])
adata_concat.obs[cell_type_key][: len(test_embed_adata)] = "To be predicted"
scGPT - INFO - match 2978/3000 genes in vocabulary of size 60697.
/usr/local/lib/python3.10/dist-packages/ipykernel/ipkernel.py:283: DeprecationWarning: 'should_run_async' will not call 'transform_cell' automatically in the future. Please pass the result to 'transformed_cell' ar
and should_run_async(code)
/usr/local/lib/python3.10/dist-packages/scgpt/model/model.py:77: UserWarning: flash-attn is not installed, using pytorch transformer instead. Set use_fast_transformer=False to avoid this warning. Installing flash-
warnings.warn(
Embedding cells: 100%| | 363/363 [03:00<00:00, 2.02it/s]
/usr/local/lib/python3.10/dist-packages/scgpt/tasks/cell_emb.py:279: ImplicitModificationWarning: Setting element `.obsm['X_scGPT']` of view, initializing view as actual.
adata.obsm["X_scGPT"] = cell_embeddings
scGPT - INFO - match 2978/3000 genes in vocabulary of size 60697.
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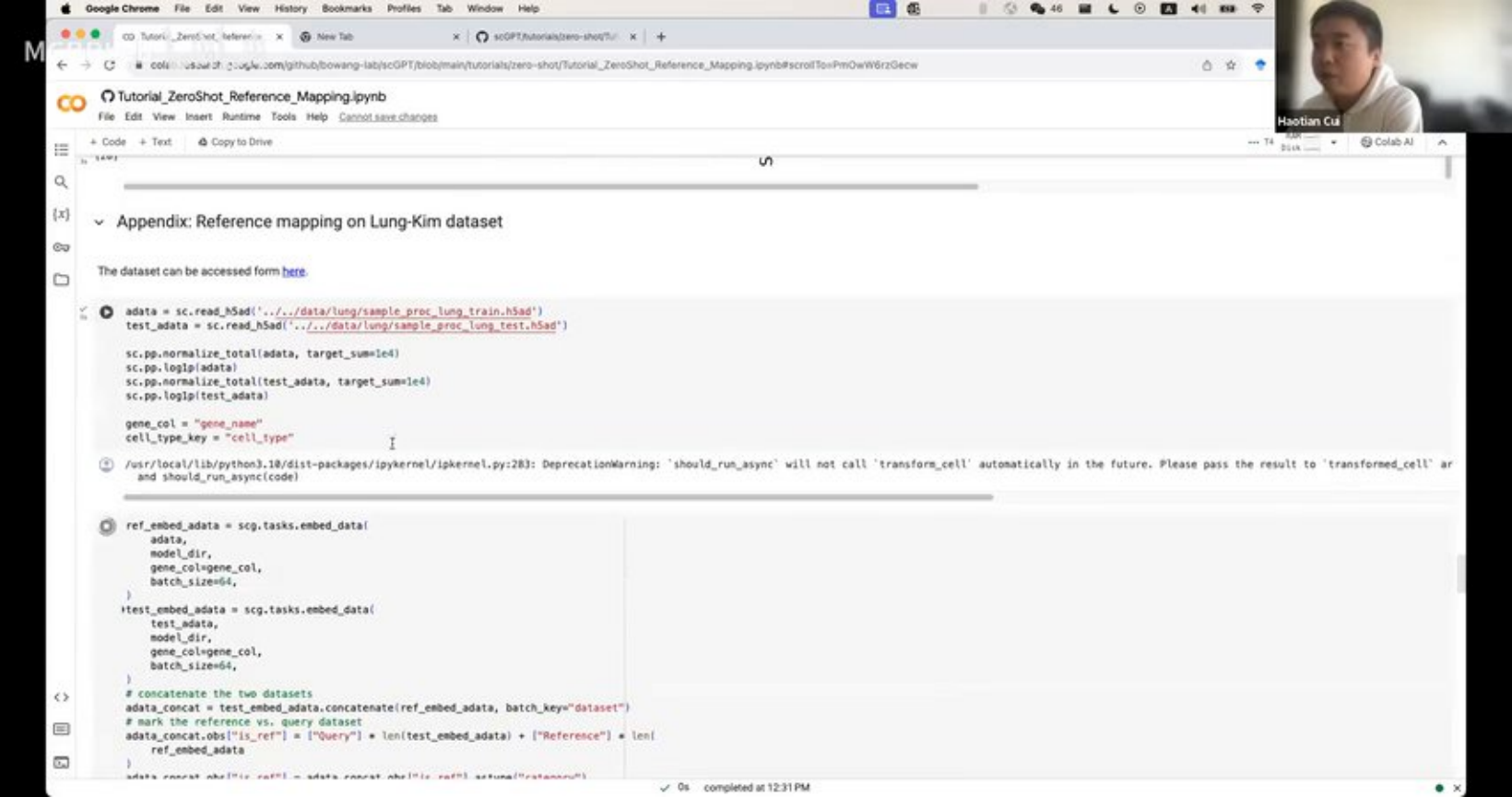
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Appendix: Reference mapping on Lung-Kim dataset
The dataset can be accessed form here.
adata = sc.read_h5ad('../../data/lung/sample_proc_lung_train.h5ad')
test_adata = sc.read_h5ad('../../data/lung/sample_proc_lung_test.h5ad')
sc.pp.normalize_total(adata, target_sum=1e4)
sc.pp.log1p(adata)
sc.pp.normalize_total(test_adata, target_sum=1e4)
sc.pp.log1p(test_adata)
gene_col = "gene_name"
cell_type_key = "cell_type"
/usr/local/lib/python3.10/dist-packages/ipykernel/ipkernel.py:283: DeprecationWarning: `should_run_async` will not call `transform_cell` automatically in the future. Please pass the result to `transformed_cell` ar
and should_run_async(code)
ref_embed_adata = scg.tasks.embed_data(
adata,
model_dir,
gene_col=gene_col,
batch_size=64,
)
test_embed_adata = scg.tasks.embed_data(
test_adata,
model_dir,
gene_col=gene_col,
batch_size=64,
)
# concatenate the two datasets
adata_concat = test_embed_adata.concatenate(ref_embed_adata, batch_key="dataset")
# mark the reference vs. query dataset
adata_concat.obs["is_ref"] = ["Query"] * len(test_embed_adata) + ["Reference"] * len(
ref_embed_adata
)
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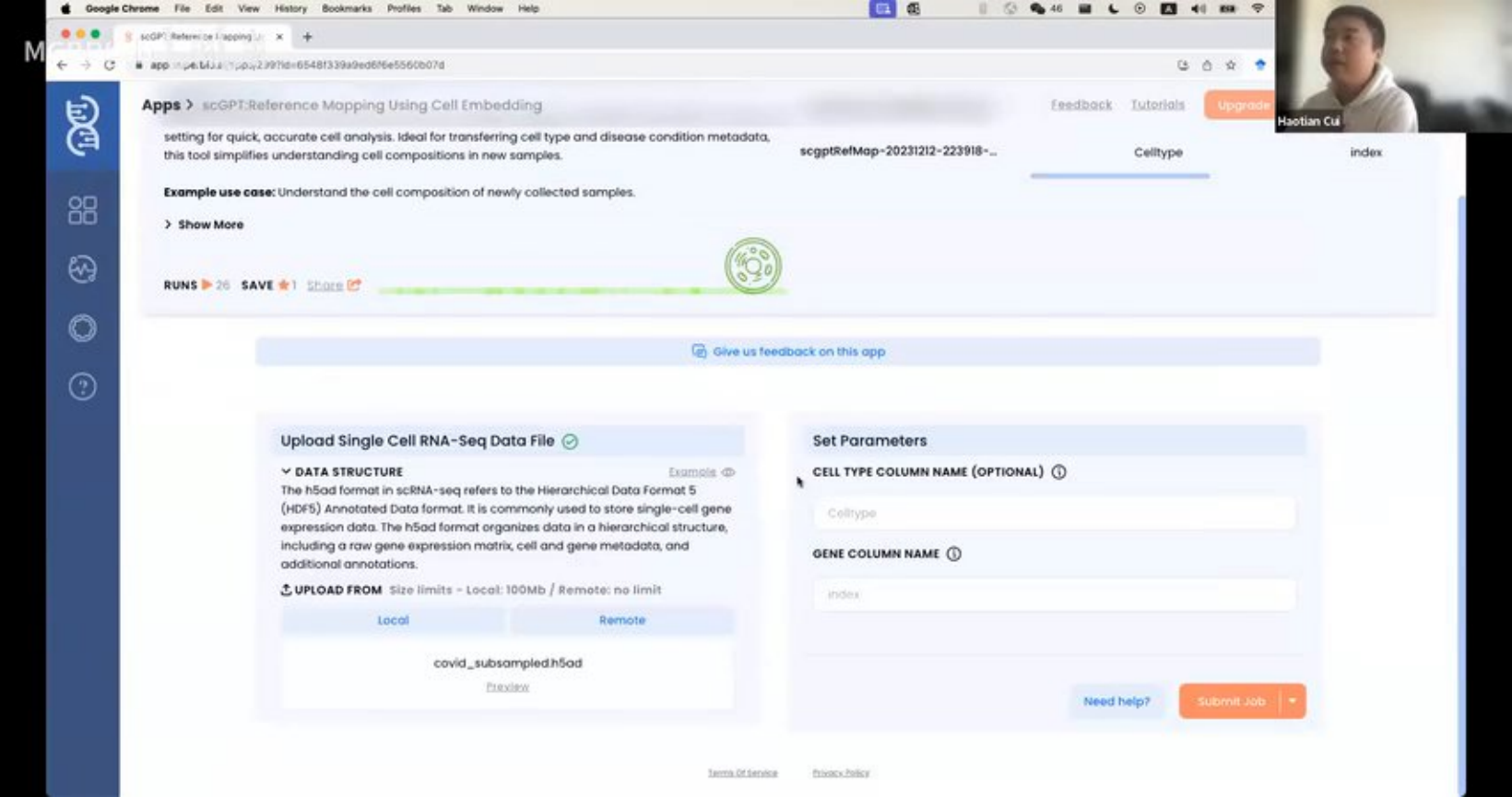
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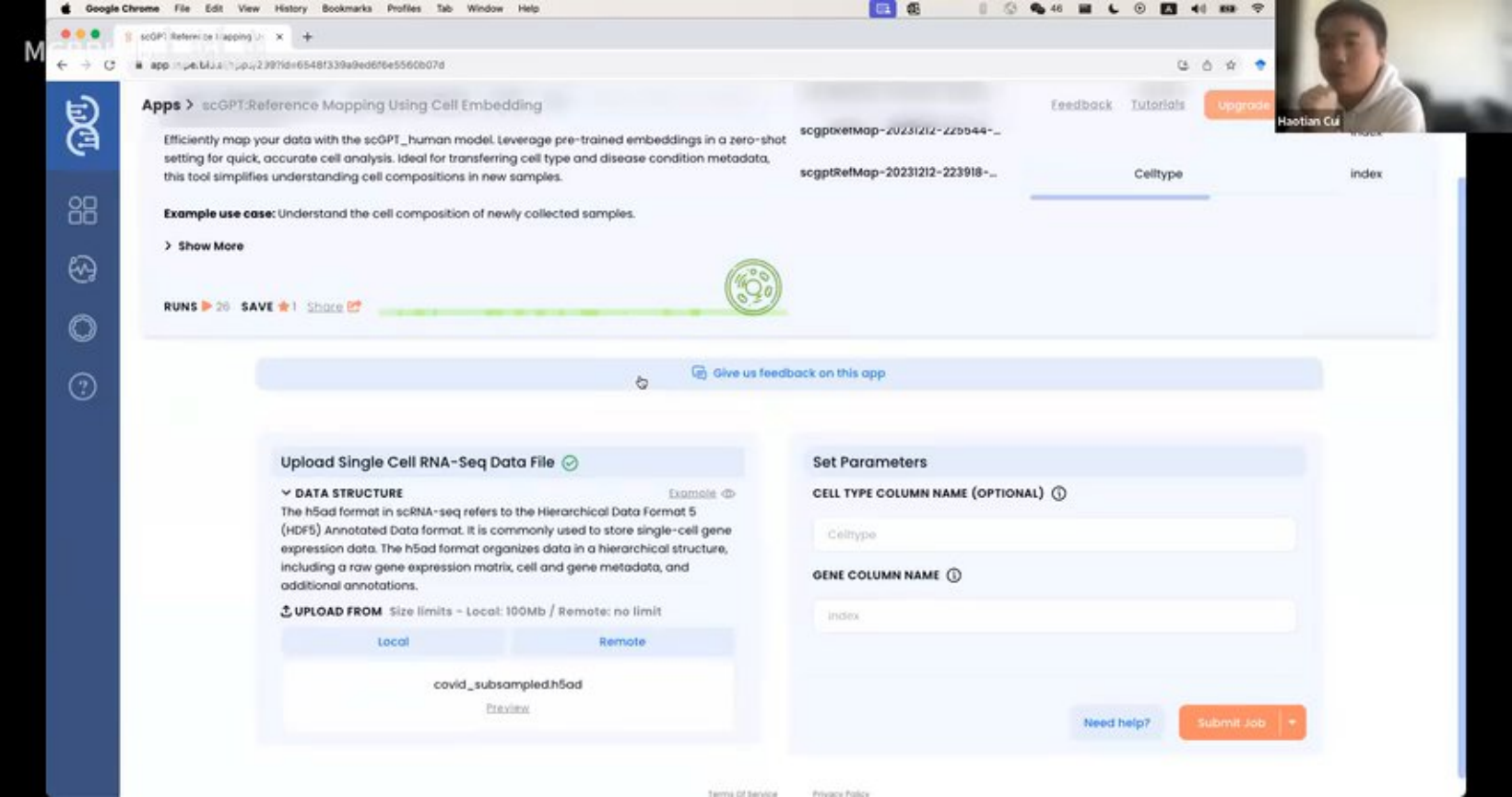
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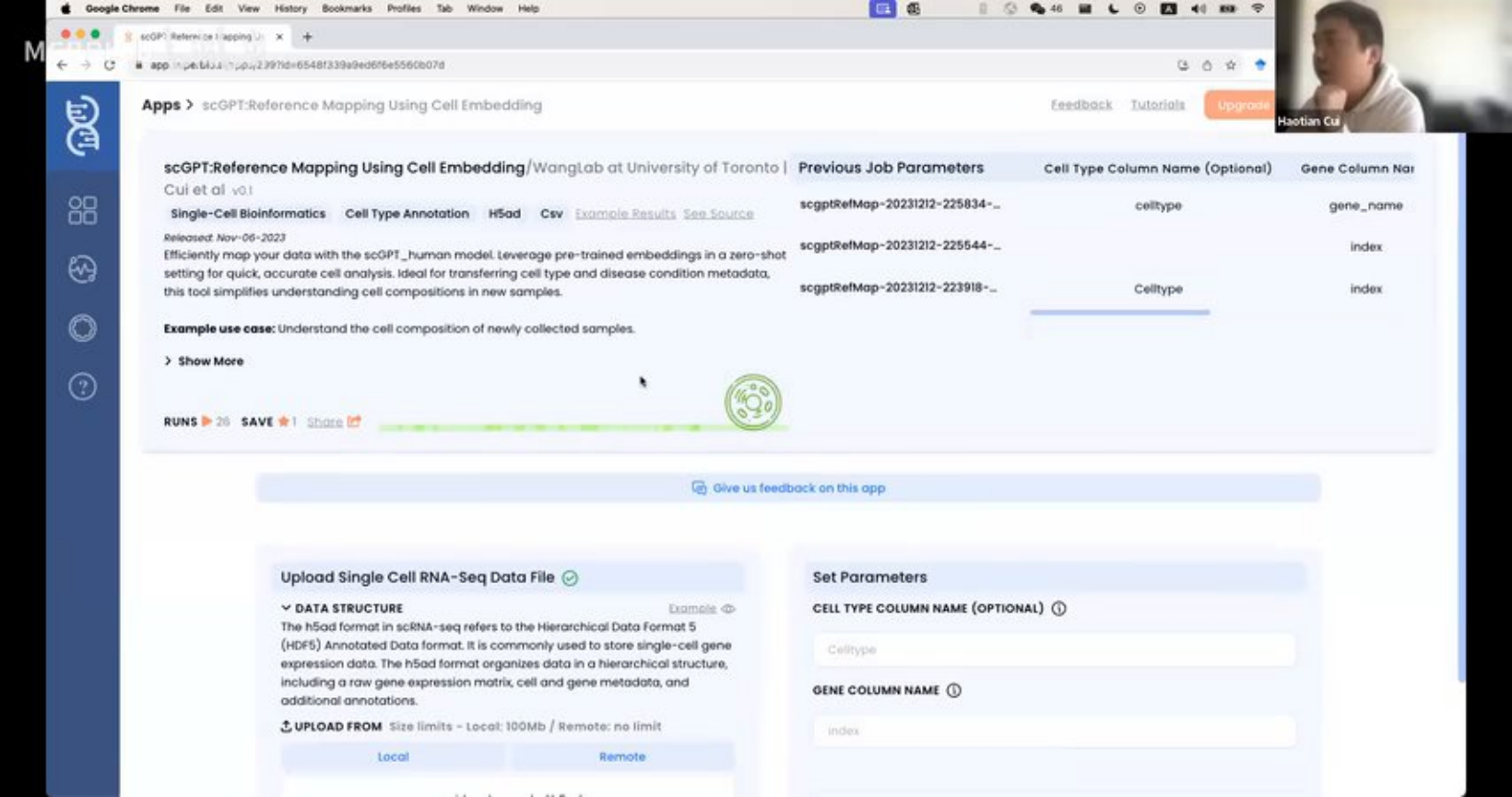
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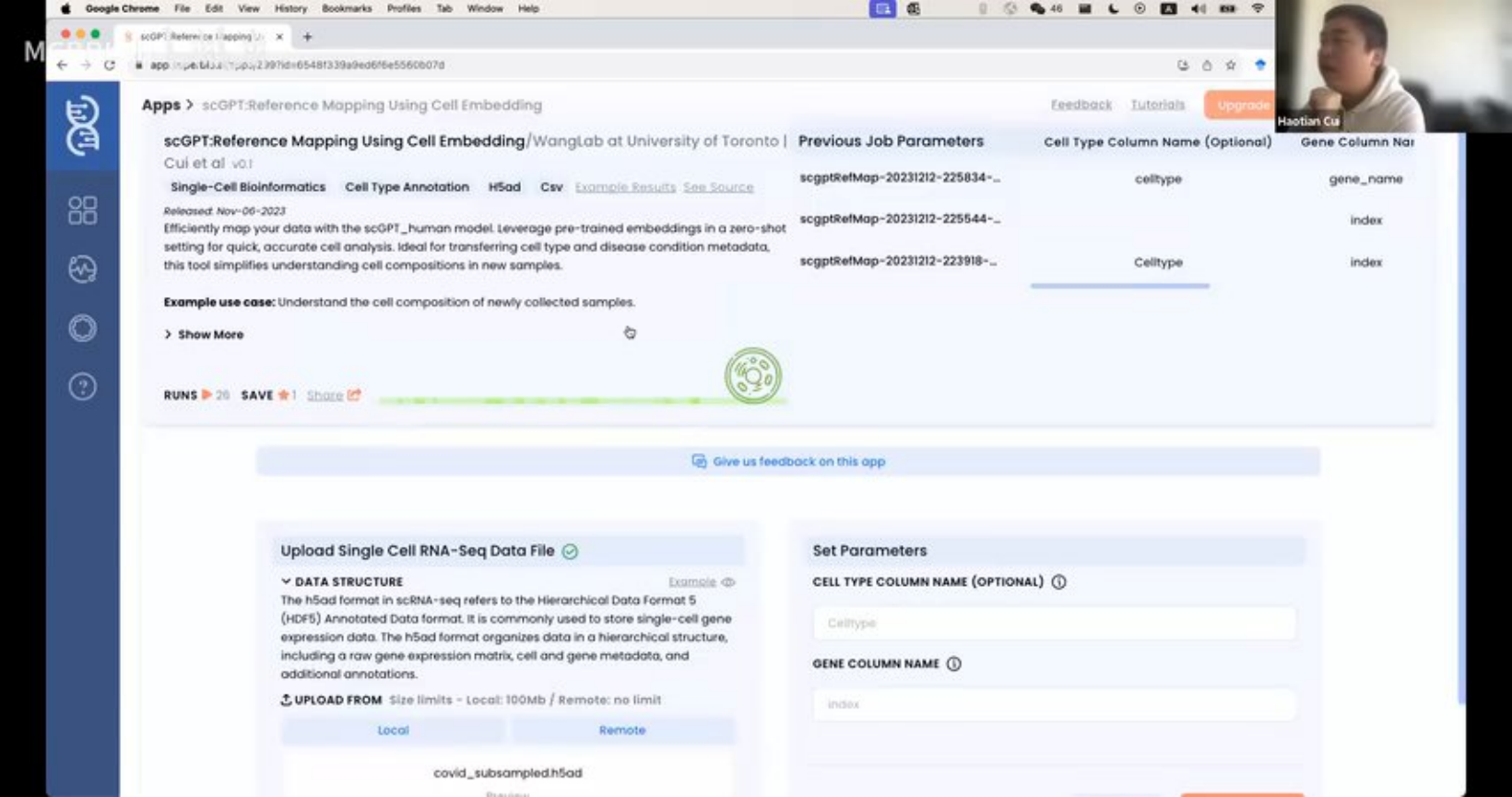
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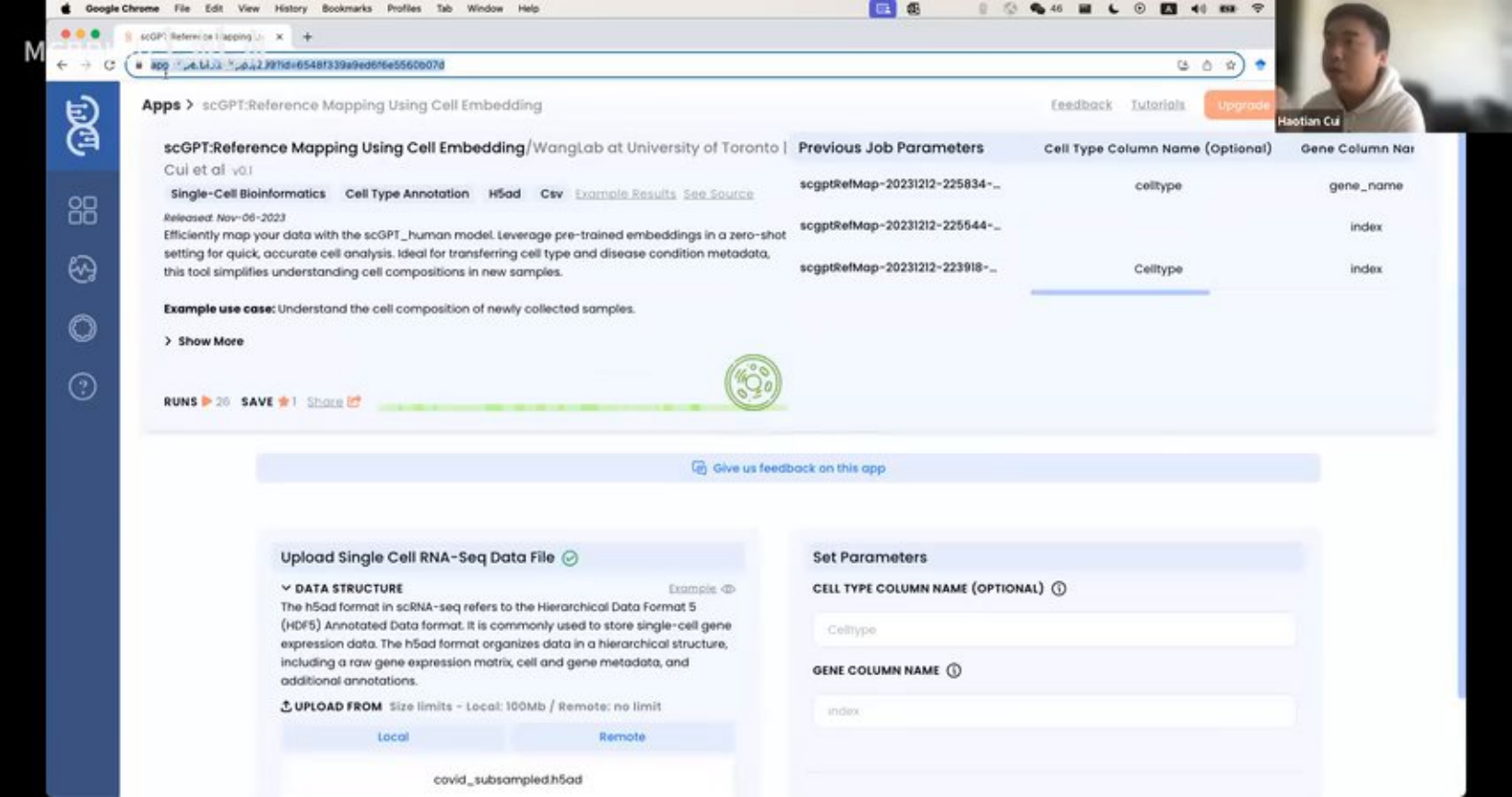
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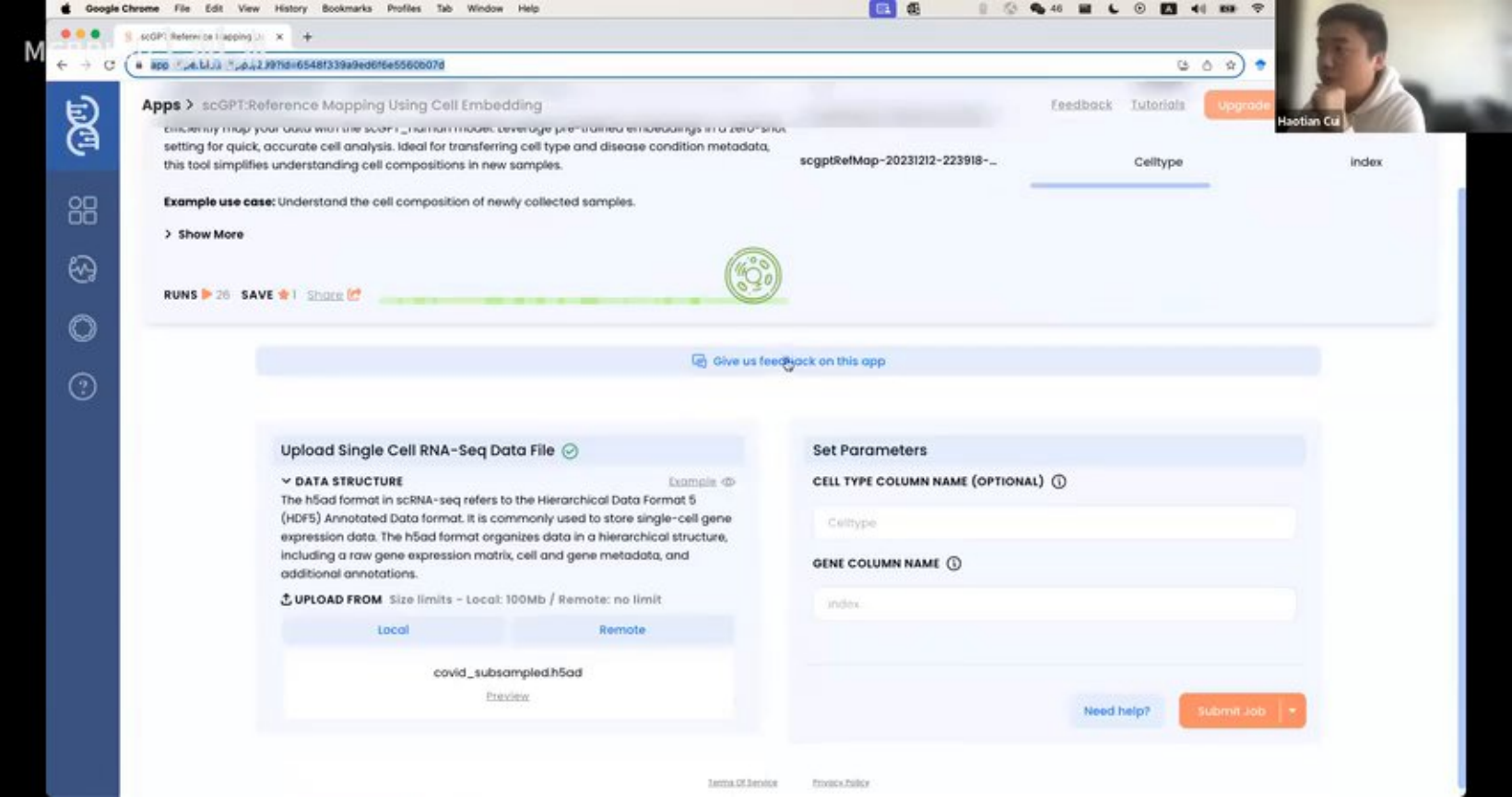
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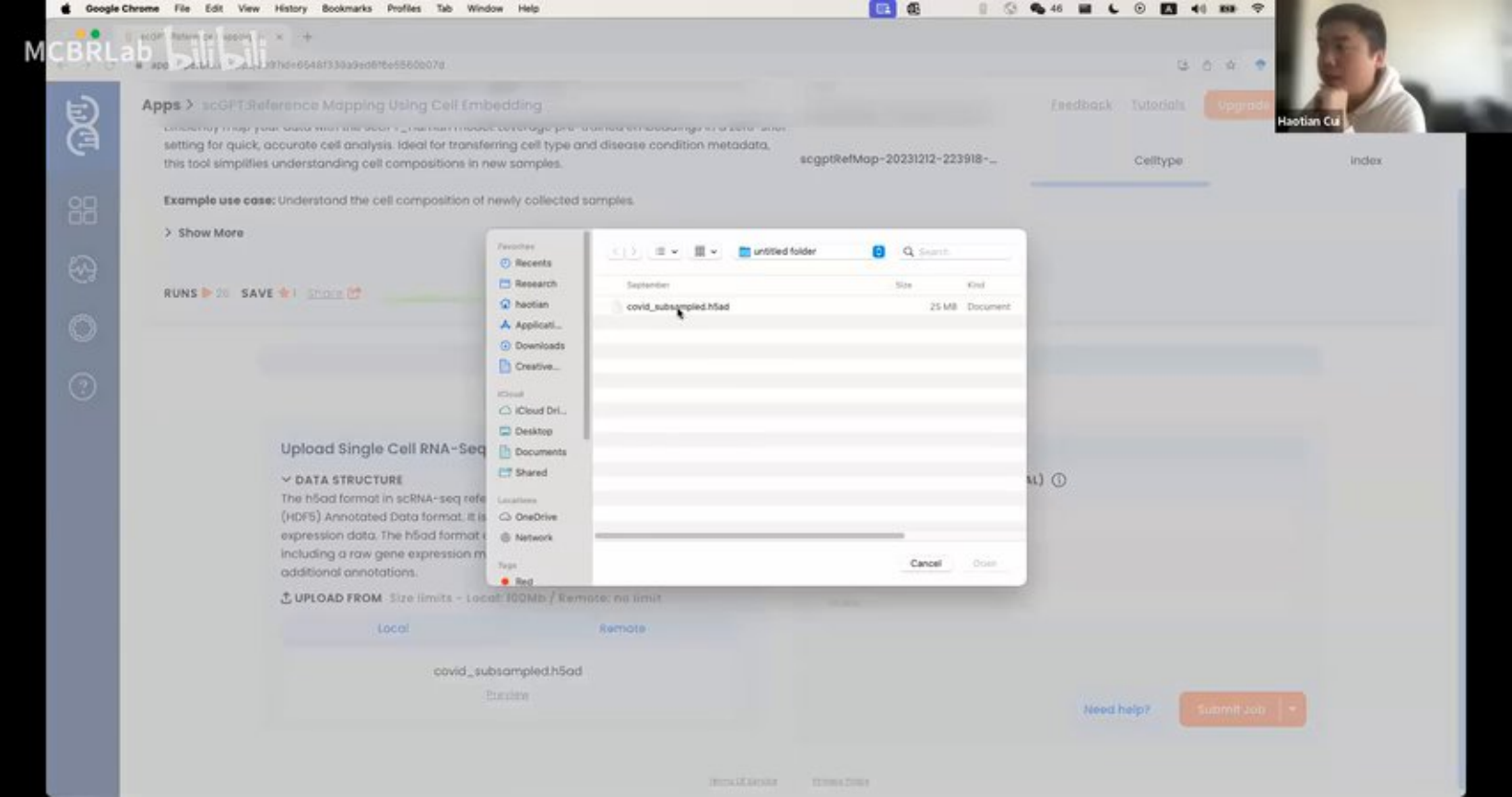
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additional annotations.
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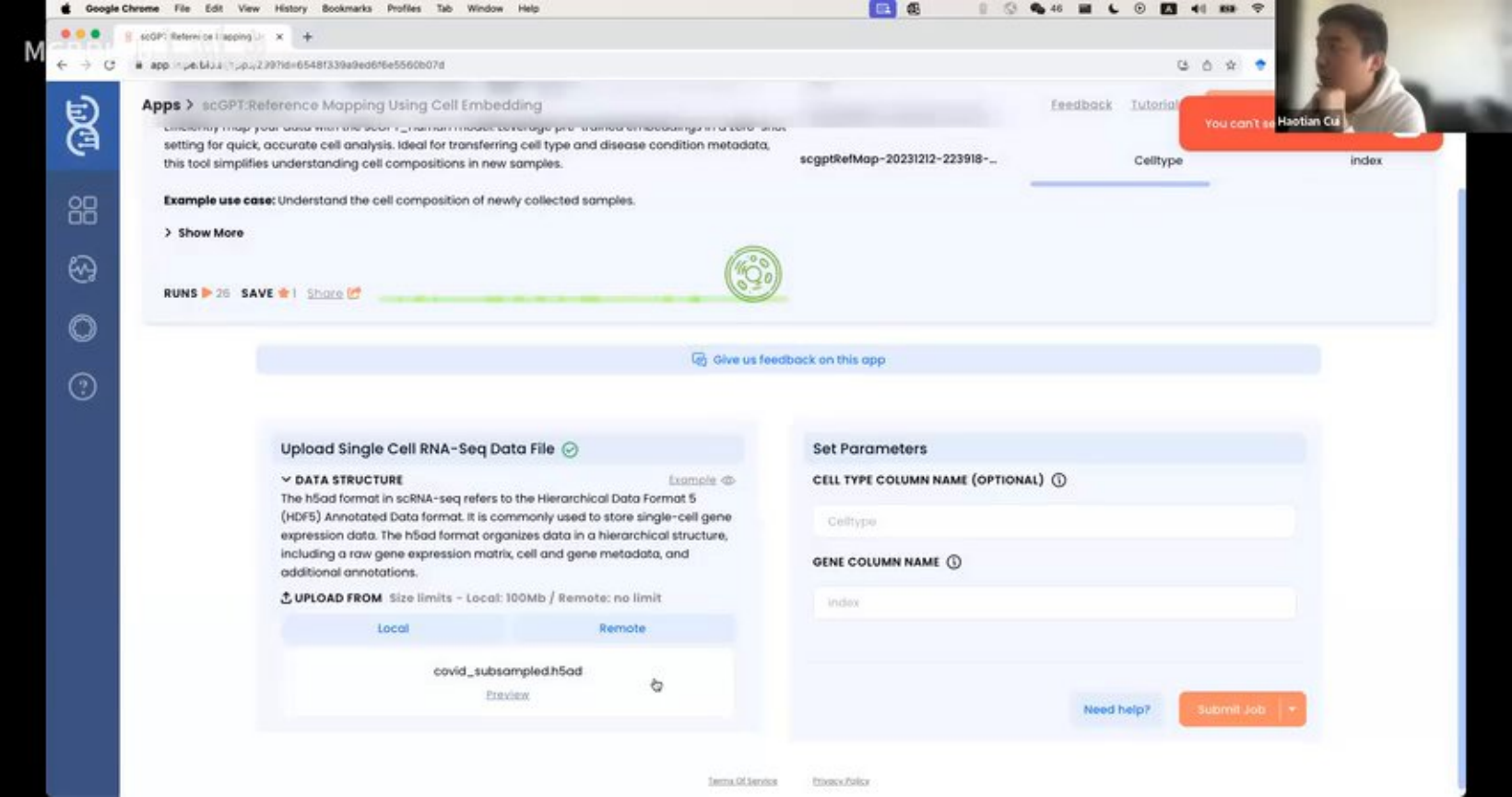
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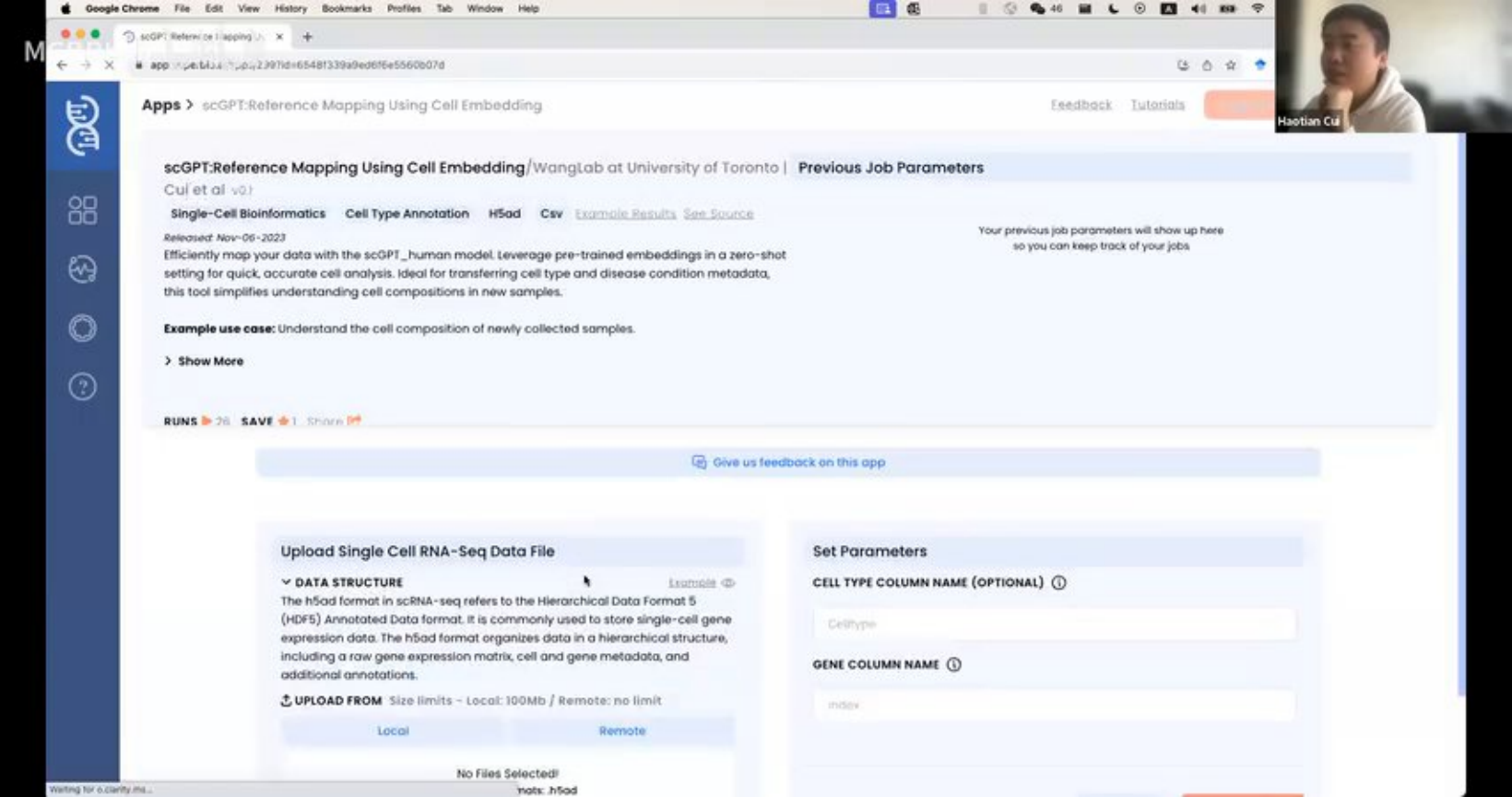
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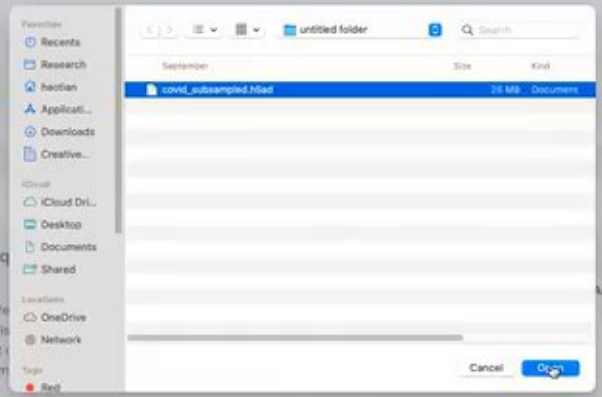

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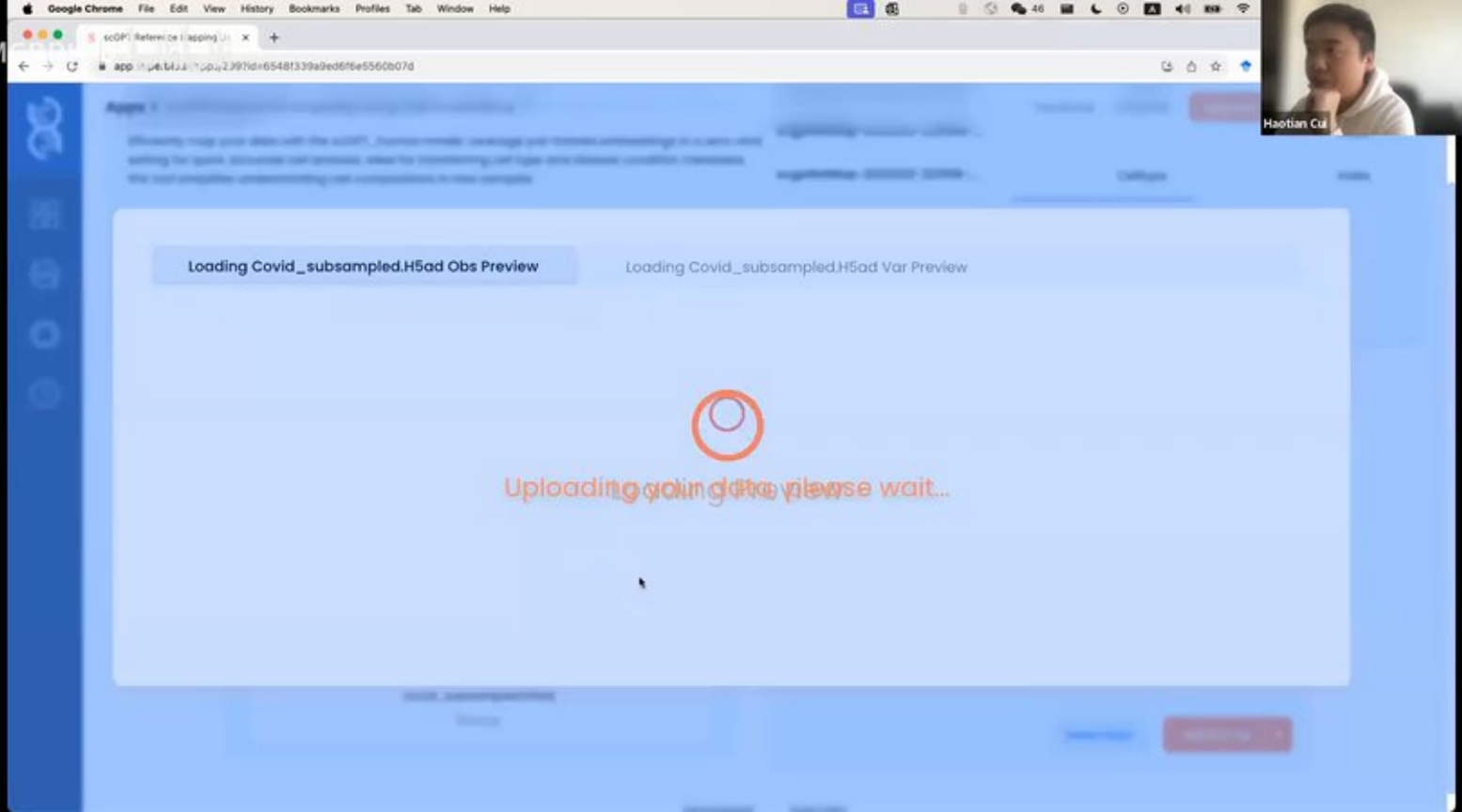
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Loading Covid_subsampled.H5ad Obs Preview
Loading Covid_subsampled.H5ad Var Preview
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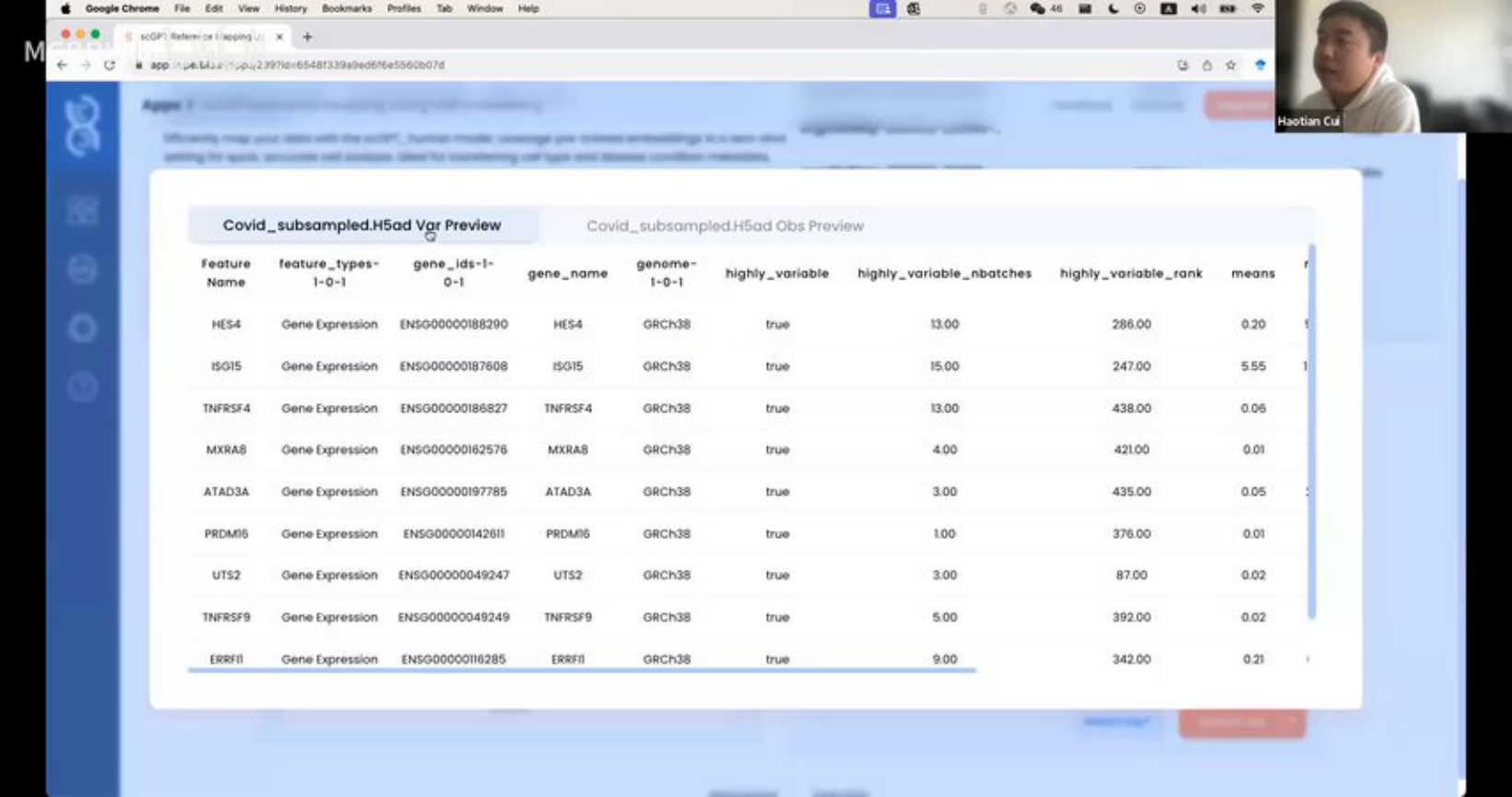
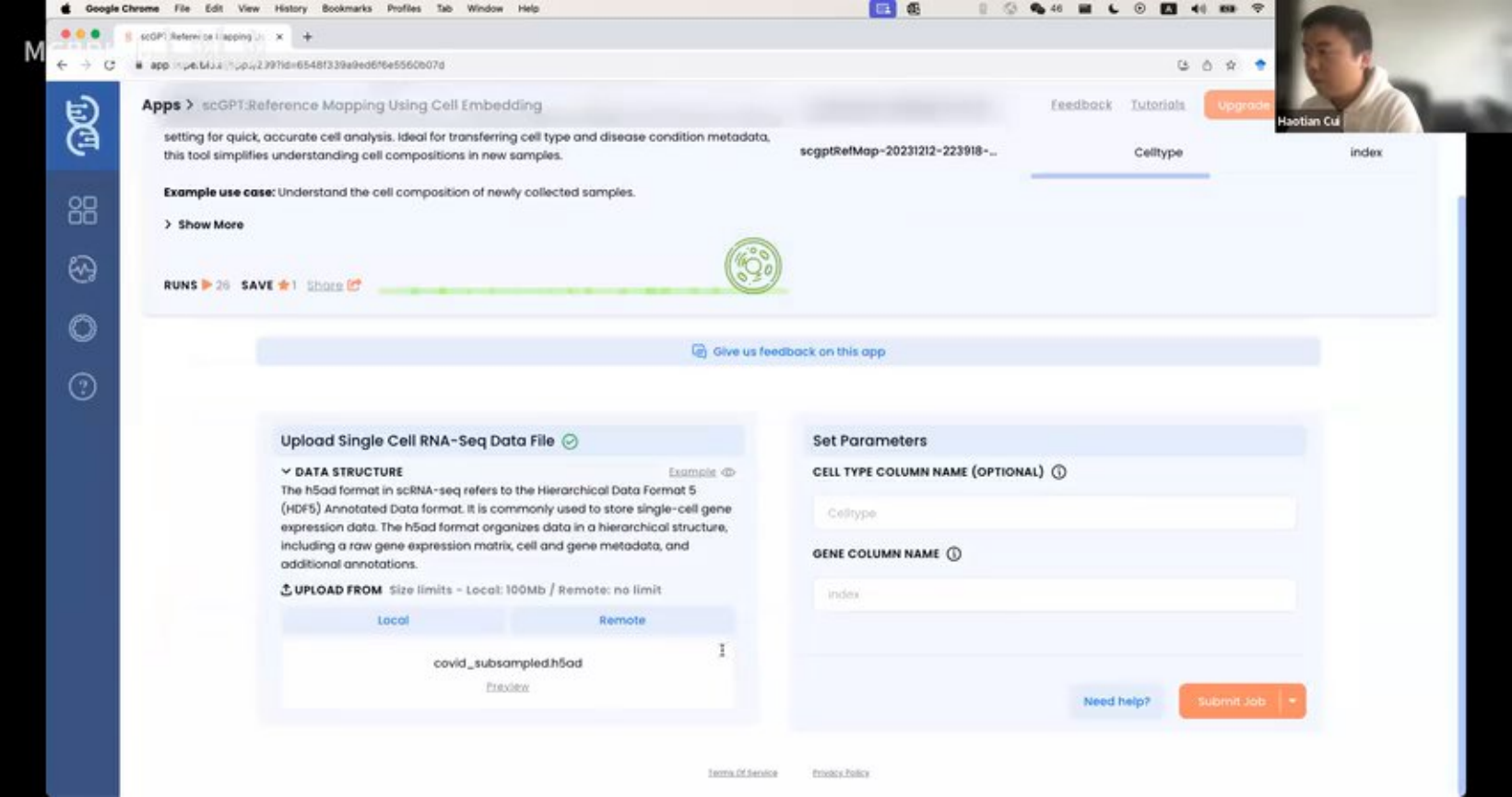


Feature Name	feature_types-1-0-1	gene_ids-1-0-1	gene_name	genome-1-0-1	highly_variable	highly_variable_nbatches	highly_variable_rank	means
HES4	Gene Expression	ENSG00000188290	HES4	GRCh38	true	13.00	286.00	0.20
ISG15	Gene Expression	ENSG00000187608	ISG15	GRCh38	true	15.00	247.00	5.55
TNFRSF4	Gene Expression	ENSG00000186827	TNFRSF4	GRCh38	true	13.00	438.00	0.06
MXRA8	Gene Expression	ENSG00000162576	MXRA8	GRCh38	true	4.00	421.00	0.01
ATAD3A	Gene Expression	ENSG00000197785	ATAD3A	GRCh38	true	3.00	435.00	0.05
PRDM16	Gene Expression	ENSG00000142611	PRDM16	GRCh38	true	1.00	376.00	0.01
UTS2	Gene Expression	ENSG00000049247	UTS2	GRCh38	true	3.00	87.00	0.02
TNFRSF9	Gene Expression	ENSG00000049249	TNFRSF9	GRCh38	true	5.00	392.00	0.02
ERRFI1	Gene Expression	ENSG00000116285	ERRFI1	GRCh38	true	9.00	342.00	0.21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Example
The h5ad format in scRNA-seq refers to the Hierarchical Data Format 5 (HDF5) Annotated Data format. It is commonly used to store single-cell gene expression data. The h5ad format organizes data in a hierarchical structure, including a raw gene expression matrix, cell and gene metadata, and additional annotations.
UPLOAD FROM Size limits - Local: 100Mb / Remote: no limit
Local
Remote
covid_subsampled.h5ad
Preview
Set Parameters
CELL TYPE COLUMN NAME (OPTIONAL)
Celltype
GENE COLUMN NAME
index
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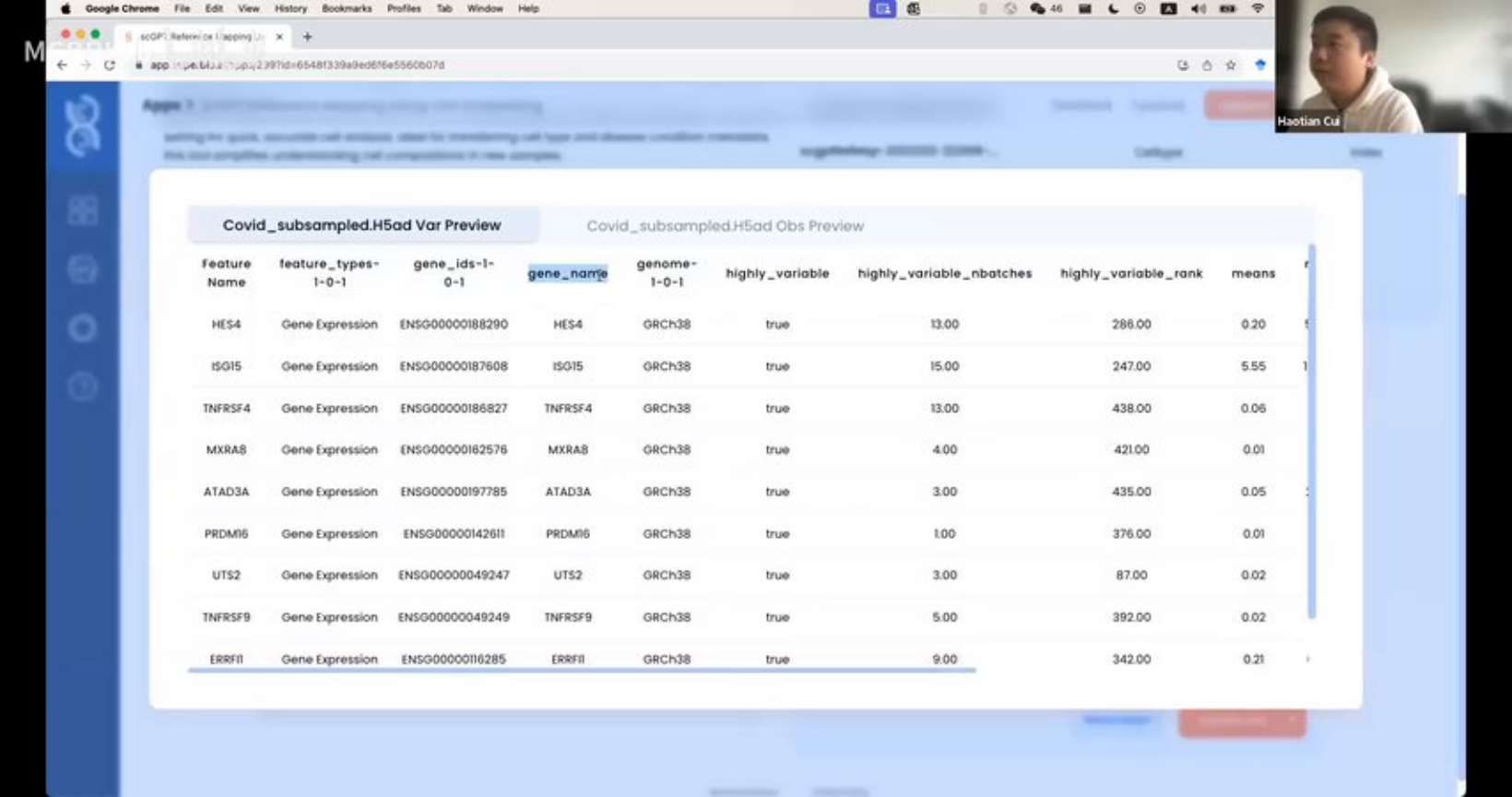

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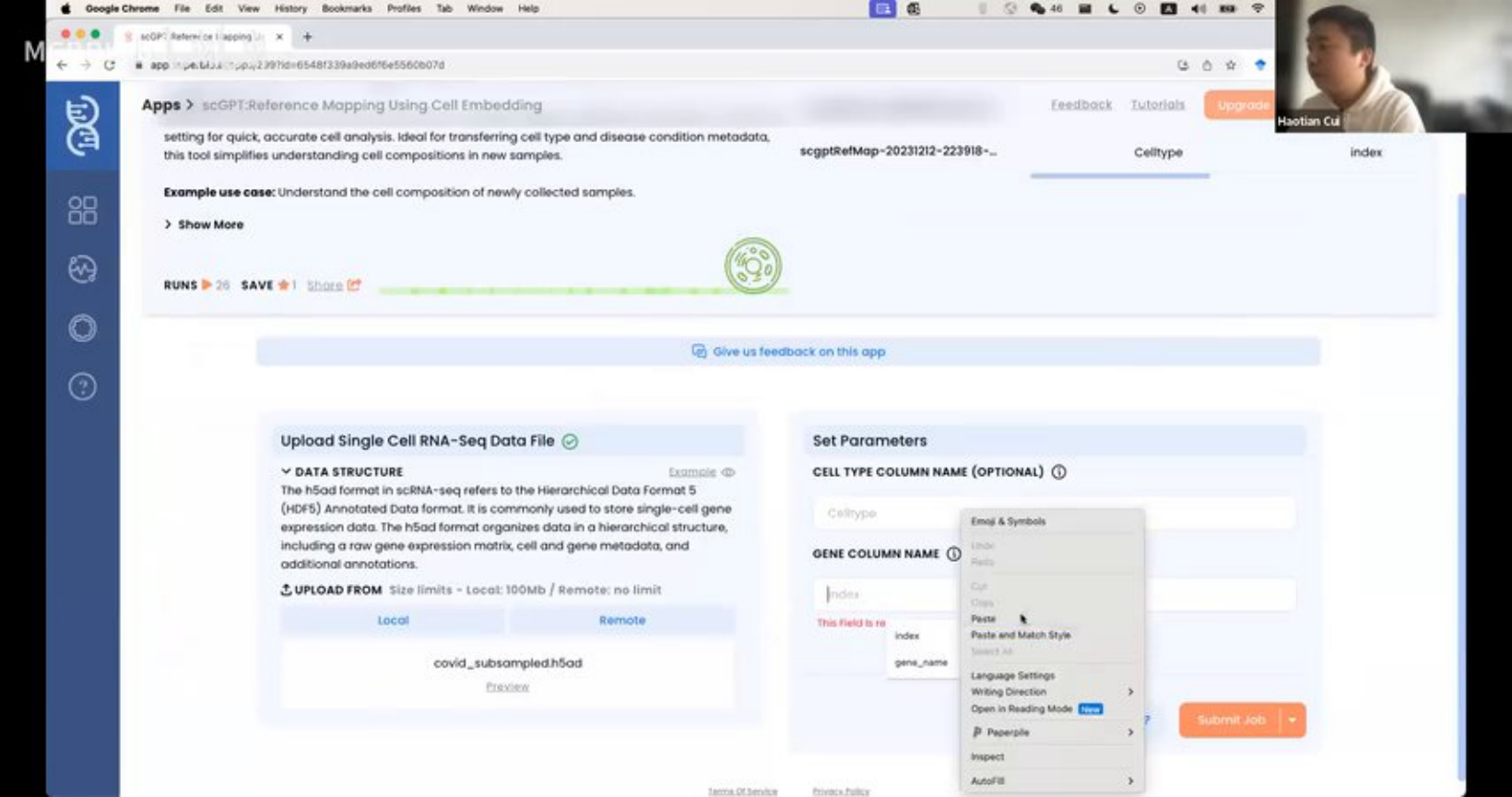
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index
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UPLOAD FROM Size limits - Local: 100Mb / Remote: no limit
Local
Remote
covid_subsampled.h5ad
Preview
Set Parameters
CELL TYPE COLUMN NAME (OPTIONAL)
Celltype
GENE COLUMN NAME
index
This field is re
index
gene_name
Emoji & Symbols
Undo
Redo
Cut
Copy
Paste
Paste and Match Style
Select All
Language Settings
Writing Direction
Open in Reading Mode
New
Paperpile
Inspect
AutoFill
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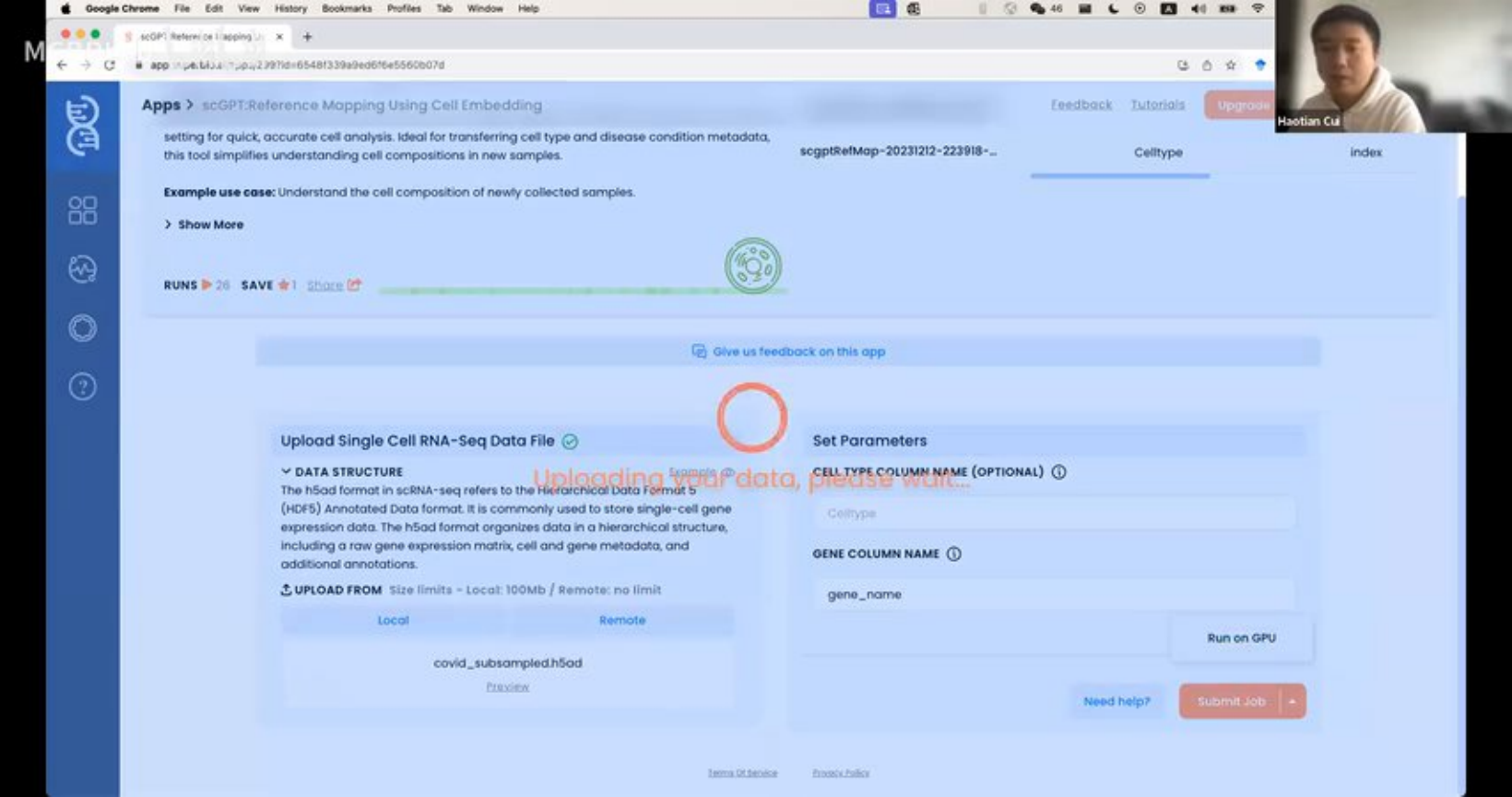
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UPLOAD FROM Size limits - Local: 100Mb / Remote: no limit
Local
Remote
covid_subsampled.h5ad
Preview
Uploading your data, please wait...
Set Parameters
CELL TYPE COLUMN NAME (OPTIONAL)
Celltype
GENE COLUMN NAME
gene_name
Run on GPU
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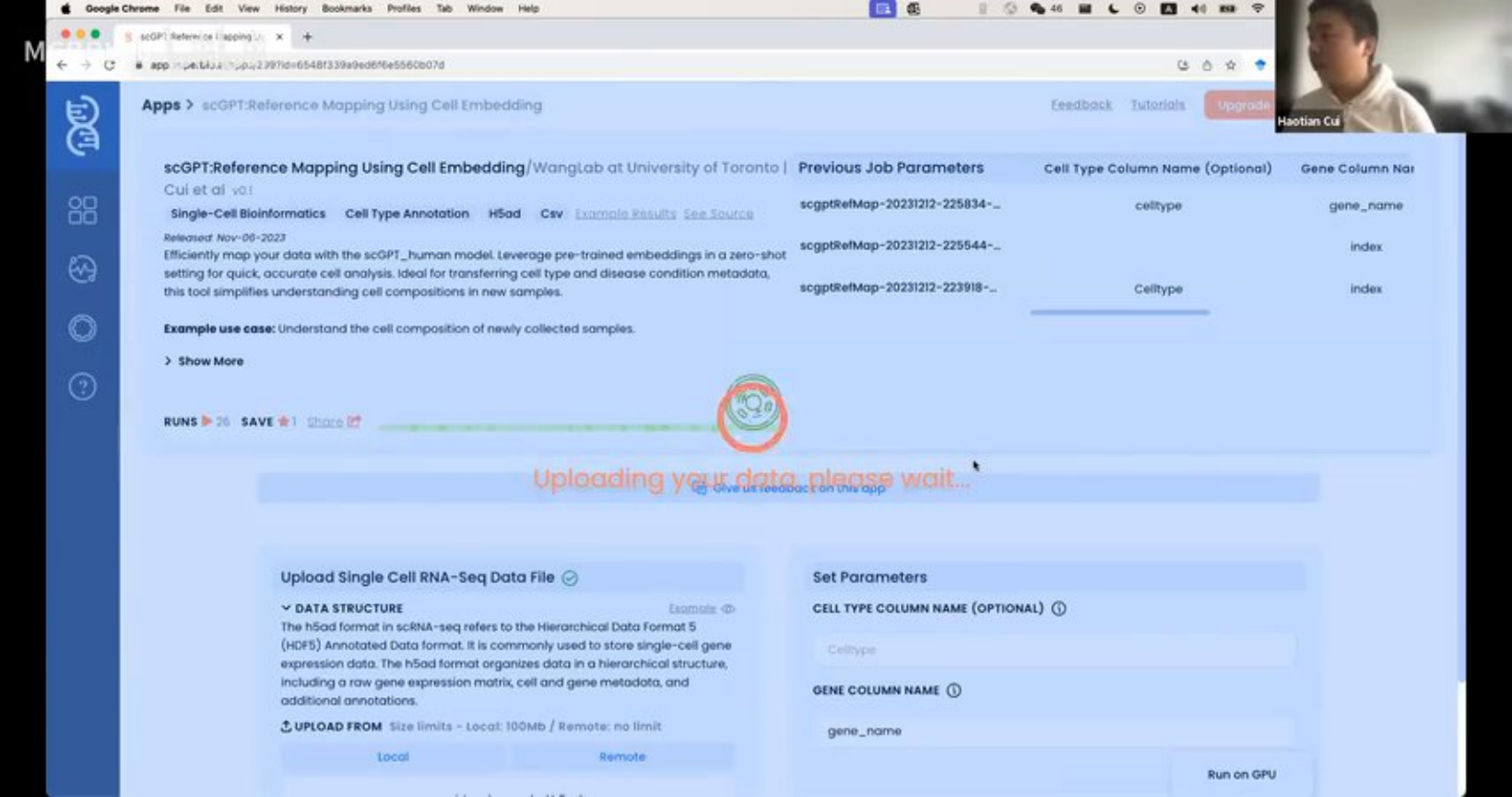
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scGPT:Reference Mapping Using Cell Embedding/WangLab at University of Toronto | Cui et al v0.1
Single-Cell Bioinformatics Cell Type Annotation H5ad Csv Example Results See Source
Released: Nov-06-2023
Efficiently map your data with the scGPT_human model. Leverage pre-trained embeddings in a zero-shot setting for quick, accurate cell analysis. Ideal for transferring cell type and disease condition metadata, this tool simplifies understanding cell compositions in new samples.
Example use case: Understand the cell composition of newly collected samples.
> Show More
Previous Job Parameters
Cell Type Column Name (Optional)
Gene Column Nar
scgptRefMap-20231212-225834-...
celltype
gene_name
scgptRefMap-20231212-225544-...
index
scgptRefMap-20231212-223918-...
Celltype
index
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DATA STRUCTURE
Example
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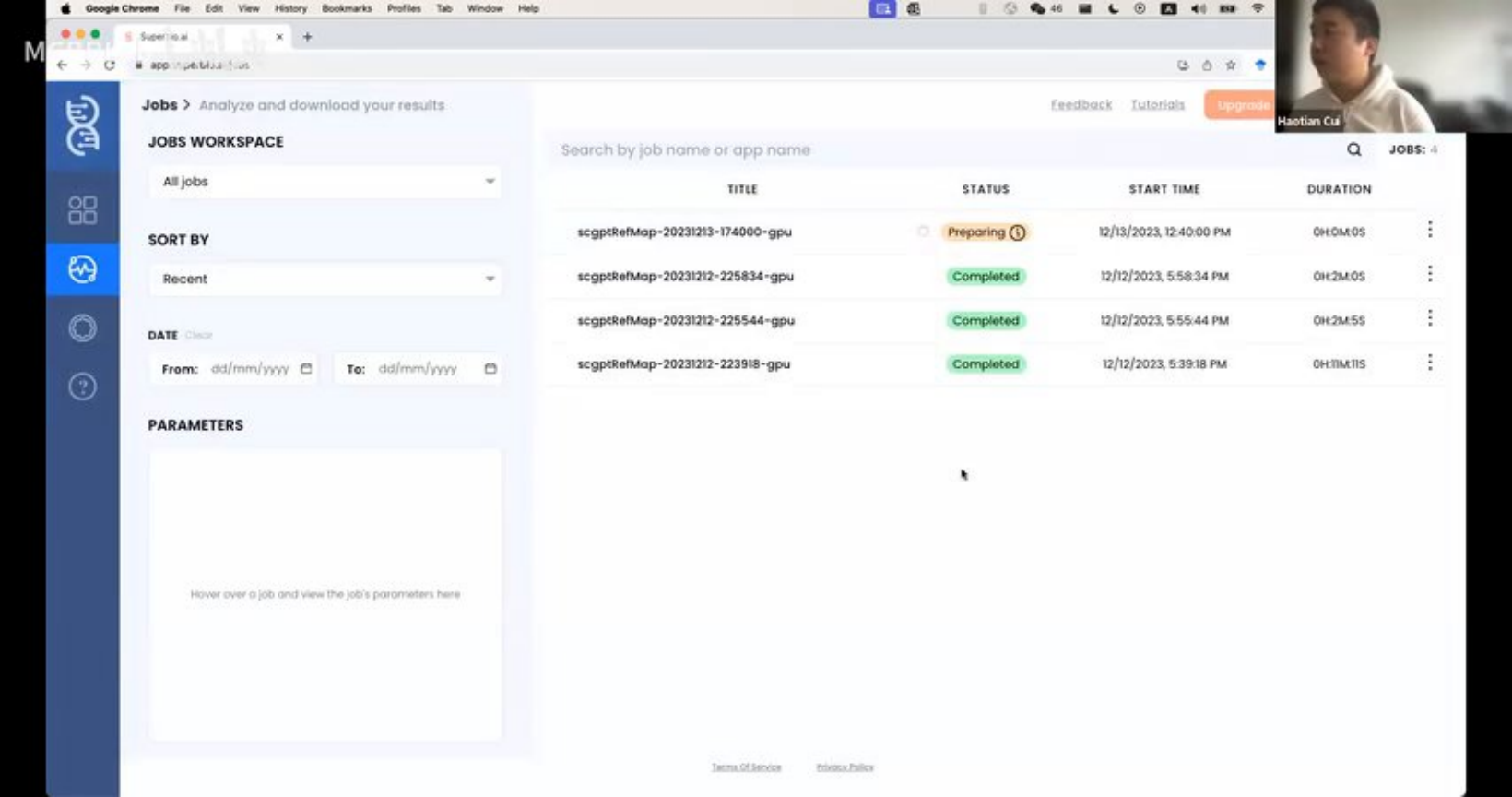
UPLOAD FROM Size limits - Local: 100Mb / Remote: no limit
Local
Remote
Set Parameters
CELL TYPE COLUMN NAME (OPTIONAL)
Celltype
GENE COLUMN NAME
gene_name
Run on GPU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From: dd/mm/yyyy
To: dd/mm/yyyy
PARAMETERS
Hover over a job and view the job's parameters here
Search by job name or app name
JOBS: 4
TITLE
STATUS
START TIME
DURATION
scgptRefMap-20231213-174000-gpu
Preparing
12/13/2023, 12:40:00 PM
0H:0M:0S
scgptRefMap-20231212-225834-gpu
Completed
12/12/2023, 5:58:34 PM
0H:2M:0S
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Completed
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0H:2M:5S
scgptRefMap-20231212-223918-gpu
Completed
12/12/2023, 5:39:18 PM
0H:11M:11S
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Results

Below, you'll find a preview of the comparison table showcasing the original labels alongside the predicted labels if the original cell type column is provided in the parameters before submitting the job. For a comprehensive view, you can download the complete

Parameters

File H5ad:	Covid_subsampled.H5ad
Cell Type Column Name (Optional):	Celltype
Gene Column Name:	Gene_name
Workflow_name:	Workflow:Yml

Actions

Download Output Files

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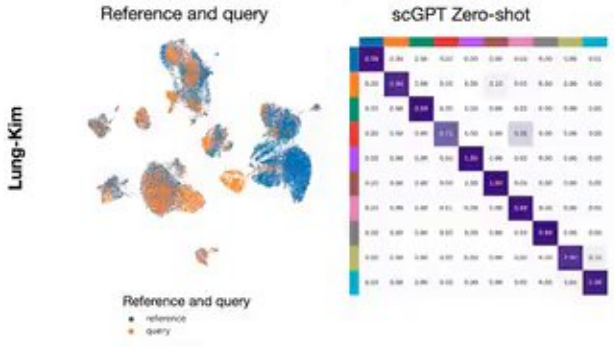
Propagated CellXGene labels (Preview)

Original Labels	CellXGene Labels
Monocytes	classical monocyte
Mast cells	mast cell
AT2	type II pneumocyte
T cell	effector memory CD8-positive, alpha-beta T cell
CD4+ T cells	CD4-positive, alpha-beta memory T cell
AT2	type II pneumocyte
Macrophages	macrophage

Contents

Zero-shot reference mapping

- We also use the embeddings in a reference mapping manner
- We split the data to simulate a setting that some of the patient cells, query set, were not annotated. Cell types were propagated from reference data set to label the query set.
- The zero-shot workflow demonstrates competitive accuracy across comparisons.



Dataset	Method	Evaluation Metrics			
		Accuracy	*Precision*	*Recall*	*MacroF1*
COVID-19	scGPT (fine-tuned)	**0.891**	**0.577**	**0.567**	**0.547**
	scGPT (zero-shot)	0.867	0.513	0.476	0.468
	Azimuth	0.878	0.515	0.418	0.444
	expiMap	0.730	0.441	0.325	0.335
Lung-Kim	scGPT (fine-tuned)	**0.974**	0.959	**0.967**	**0.962**
	scGPT (zero-shot)	0.968	**0.970**	0.933	0.948
	Azimuth	0.970	0.957	0.962	0.959
	expiMap	0.920	0.940	0.846	0.878

Going forward

- Zero-shot can be promising, we are going to provide further updates for the scenario:
  - Hierarchical cell type labeling of reference mapping from atlas
  - Going to provide new checkpoint specifically for zero-shot cell embeddings
  - Zero-shot applications using gene embeddings
  - Others

MCBRLab

Acknowledgement

Thank you!

scGPT codebase: https://github.com/bowang-lab/scGPT.

Sincere gratitude to collaborators: Chloe Wang, Hassaan Maan, Kuan Pang, Fengning Luo, Dr. Lin Zhang, Dr. Nan Duan, and Dr. Bo Wang

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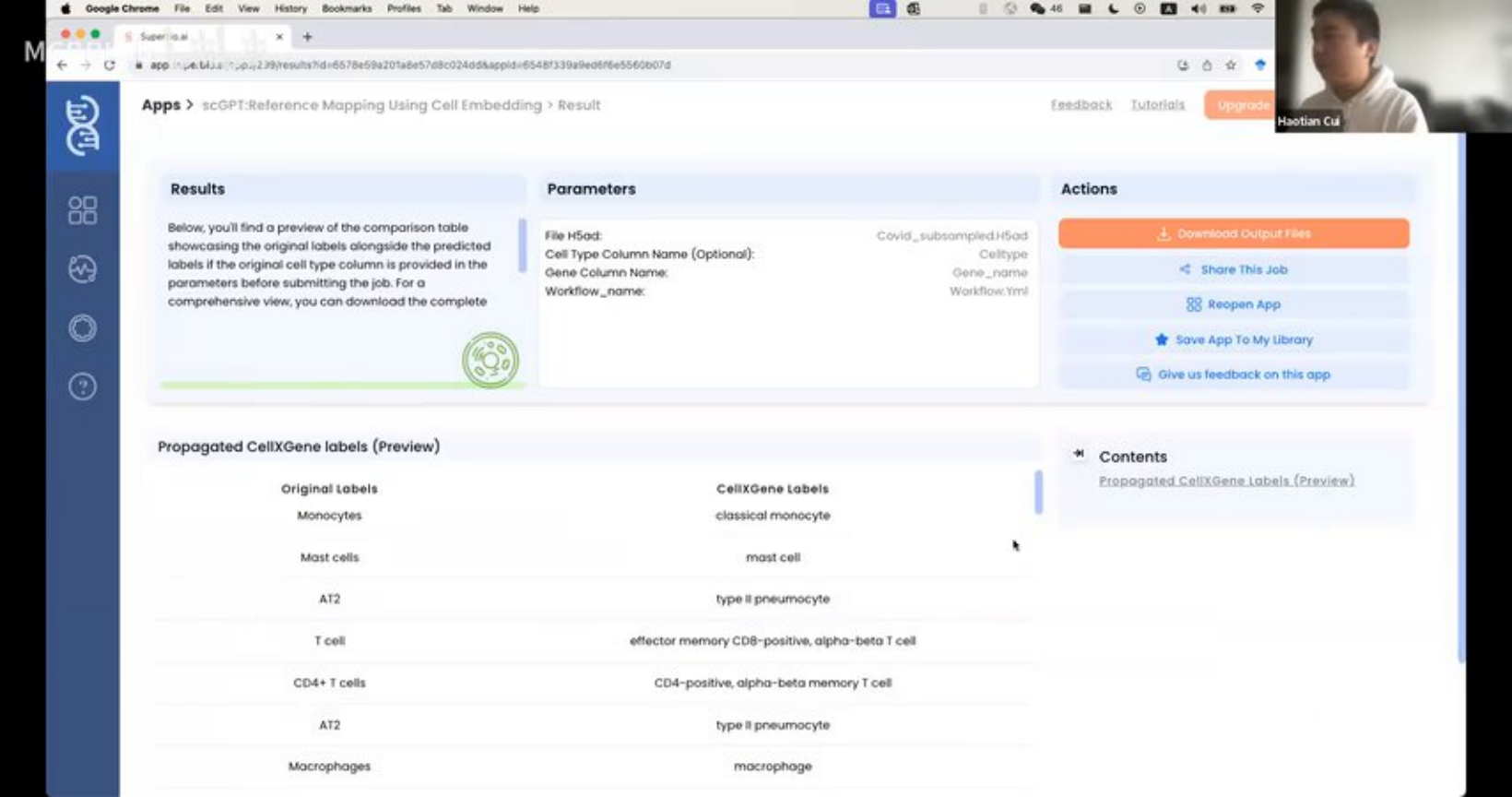
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Results
Below, you'll find a preview of the comparison table showcasing the original labels alongside the predicted labels if the original cell type column is provided in the parameters before submitting the job. For a comprehensive view, you can download the complete
Parameters
File H5ad: Covid_subsampled.H5ad
Cell Type Column Name (Optional): Celltype
Gene Column Name: Gene_name
Workflow_name: Workflow.Yml
Actions
Download Output Files
Share This Job
Reopen App
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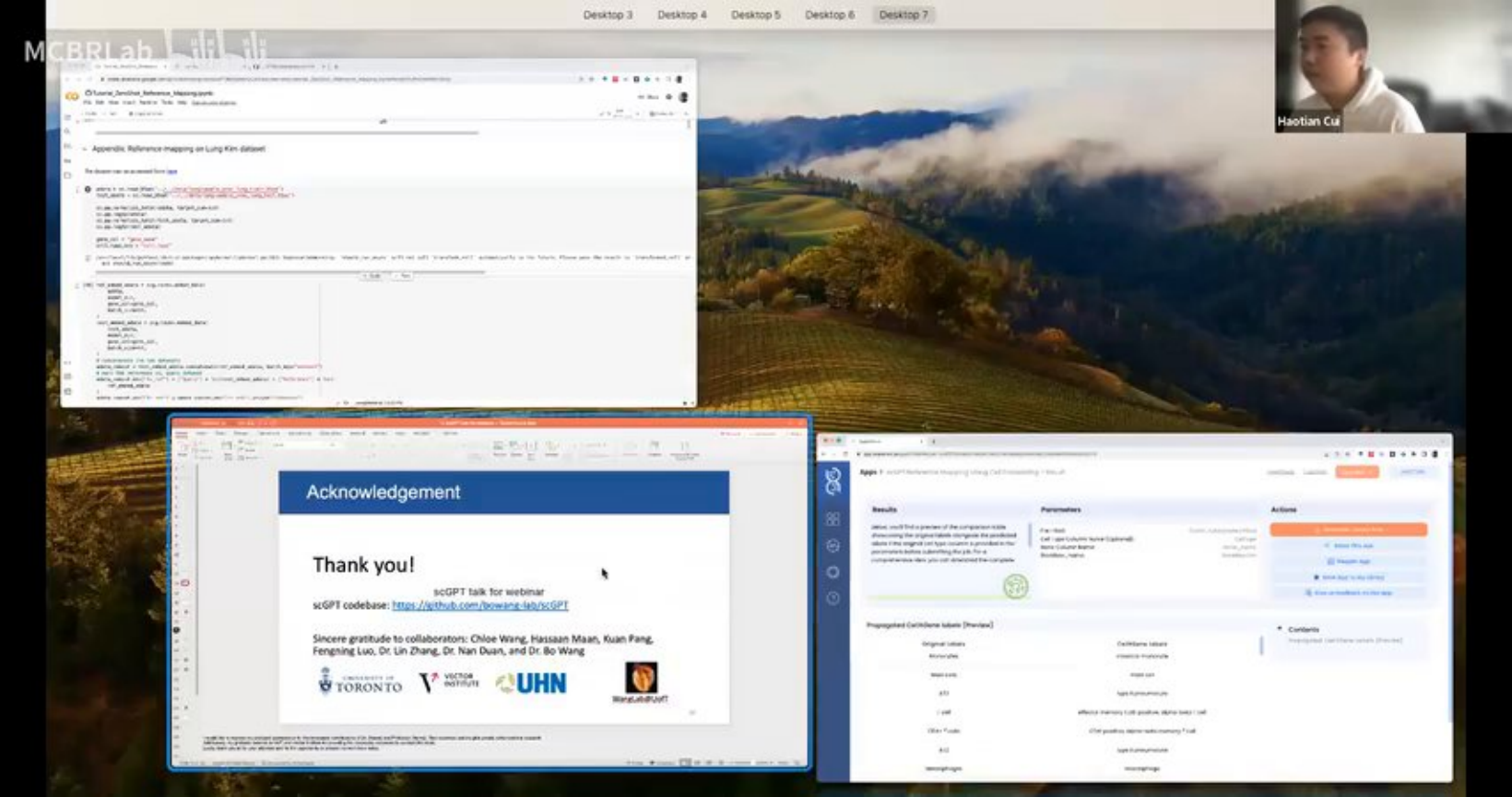
Give us feedback on this app
Propagated CellXGene labels (Preview)
Original Labels
CellXGene Labels
Monocytes
classical monocyte
Mast cells
mast cell
AT2
type II pneumocyte
T cell
effector memory CD8-positive, alpha-beta T cell
CD4+ T cells
CD4-positive, alpha-beta memory T cell
AT2
type II pneumocyte
Macrophages
macrophage
Contents
Propagated CellXGene Labels (Preview)


Desktop 3
Desktop 4
Desktop 5
Desktop 6
Desktop 7
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Appendix: Reference mapping on Lung Kim dataset
Acknowledgement
Thank you!
scGPT talk for webinar
scGPT codebase: https://github.com/bowang-lab/scGPT
Sincere gratitude to collaborators: Chloe Wang, Hassaan Maan, Kuan Pang, Fengning Luo, Dr. Lin Zhang, Dr. Nan Duan, and Dr. Bo Wang
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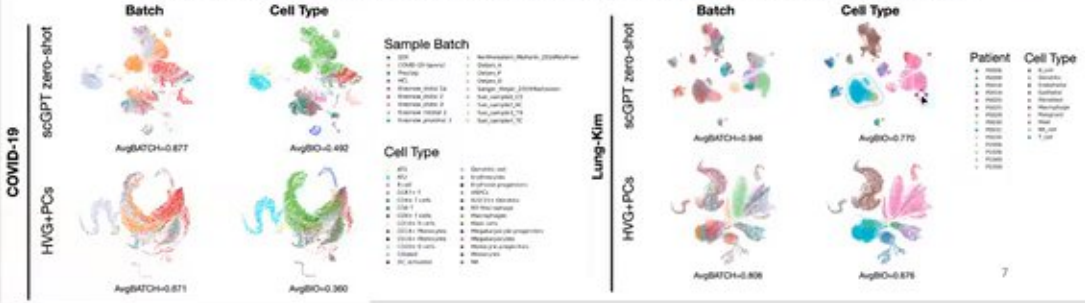
Parameters
Actions
Contents

Zero-shot applications

- **Zero-shot**, meaning using the pretrained model to generate embeddings for new data, without any further training, **much faster, more accessible**
- UMAP of zero-shot embeddings on two disease datasets, compared to HVGs
  - Considerable ability to distinguish cell types
  - Note the pretraining process is not designed for mitigating technical batch effects



Have been working new extensions exploring the possibility of zero-shot applications. Here, I'd like to share some new results

Particularly want to mention the influence of pretraining,
so of the technical info is actually signals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