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A4 Report
November 5, 2025

Task 1: Manually complete a benchmark

For this task, I opted to choose a **feature engineering and deep learning** task, since I'm most familiar with this area of data science/machine learning. Specifically, my task was as follows:

> "Train a multitask model on the Clintox dataset to predict a drug's toxicity and FDA approval status. Save the test set predictions, including the SMILES representation of drugs and the probability of positive labels, to "pred_results/clintox_test_pred.csv"."

Additionally, I was given the following domain information:

> 1. *On the task*: The ClinTox dataset contains drugs approved by the US Food and Drug Administration (FDA) and drugs that have failed clinical trials for toxicity reasons. The dataset includes two binary classification tasks for 1491 drug compounds with known chemical structures: (1) clinical trial toxicity (or absence of toxicity) and (2) FDA approval status. This requires developing a model with two binary classification heads each determining the label of its respective task based on the molecular structure. Use `MultitaskClassifier` model from the deepchem library.
> 2. *On featurization*: To represent the molecular structure, use Extended-Connectivity Fingerprints (ECFPs) featurization in deepchem. ECFPs are circular topological fingerprints that represent the presence of particular substructures and stereochemical information.

The input data for this task also had the chemical structure in Simplified Molecular Input Line Entry System (SMILES) format, which, according to Wikipedia, "is a specification in the form of a line notation for describing the structure of chemical species using short ASCII strings." It seems my job is to encode this string data as a vector representation (analogous to a word embedding) for the downstream modeling task.

In order to featurize the input SMILES sequence date, the task recommends using Extended-connectivity fingerprints (ECFPs) featurization available through the deepchem package. According to the chemistry journal ACS Publications, ECFPs are a way of encoding chemical sequences with a vector representation for numerical modeling tasks. I looked at deepchem's documentation for ECFPs (and other featurizers), which are implemented through the CircularFingerprint class. According to the documentation, an ECFP encoding is analogous to a Bag-of-Words encoding you might see in NLP data.

Additionally, in the domain knowledge, they let us know to use a MultitaskClassifier from deepchem's library, so I looked up the official documentation. The MultitaskClassifier is essentially just a multi-layer perceptron implemented in familiar sklearn syntax.

The data for this task comes from the original repo corresponding to the problem: https://github.com/anikaliu/CAMDA-DILI

I spent approximately **1.5 hours total** on this task:

- 30 mins doing background research on deepchem, SMILES, and chemical embeddings
- 1 hour to preprocess the data, train, and tune my models on each prediction task

I began by loading in the dataset and encoding the SMILES encodings as BoW-analogous embeddings via ECFP:

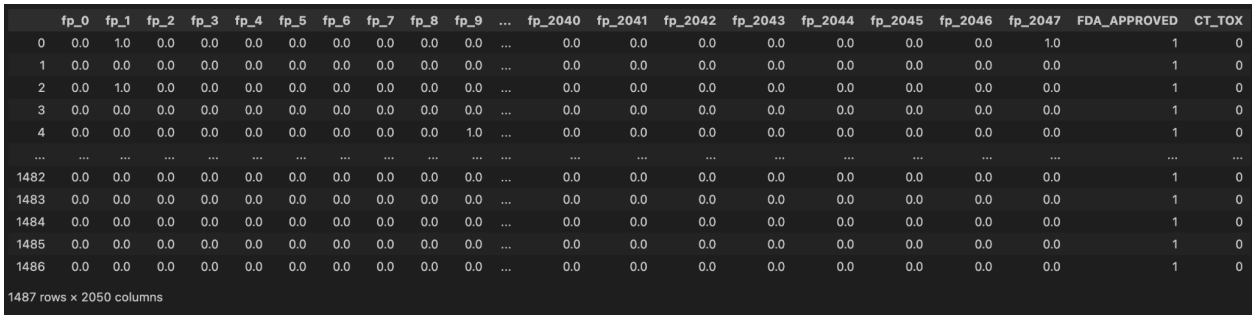
```
import pandas as pd
import numpy as np
import warnings
warnings.filterwarnings("ignore")

clintox = pd.read_csv("data/clintox.csv")
clintox
```

	smiles	FDA_APPROVED	CT_TOX
0	*C(=O)[C@H](CCCCNC(=O)OCCOC)NC(=O)OCCOC	1	0
1	[C@@H]1([C@@H]([C@@H]([C@H]([C@@H]([C@@H]1Cl)C...	1	0
2	[C@H]([C@@H]([C@@H](C(=O)[O-])O)O)([C@H](C(=O)...	1	0
3	[H]/[NH+]=C(/C1=CC(=O)/C(=C\C=c2ccc(=C([NH3+])...	1	0
4	[H]/[NH+]=C(\N)/c1ccc(cc1)OCCCCCOc2ccc(cc2)/C(...	1	0
...	...	...	...
1486	O[Si](=O)O	1	0
1487	O=[Ti]=O	1	0
1488	O=[Zn]	1	0
1489	OCl(=O)(=O)=O	1	0
1490	S=[Se]=S	1	0

1491 rows × 3 columns

```
import deepchem as dc
from rdkit import Chem

featurizer = dc.feat.CircularFingerprint(size=2048, radius=4)
features = featurizer.featurize(clintox["smiles"])
valid_idx = [i for i, f in enumerate(features) if f.shape[0] == 2048]
```

```
valid_features = [features[i] for i in valid_idx]
valid_clintox = clintox.iloc[valid_idx].reset_index(drop=True)

features_2d = np.vstack(valid_features)
fp_cols = [f"fp_{i}" for i in range(features_2d.shape[1])]
fingerprint_df = pd.DataFrame(features_2d, columns=fp_cols)
label_df = valid_clintox[["FDA_APPROVED", "CT_TOX"]]
clintox_fp_df = pd.concat([fingerprint_df, label_df], axis=1)
clintox_fp_df
```



	fp_0	fp_1	fp_2	fp_3	fp_4	fp_5	fp_6	fp_7	fp_8	fp_9	...	fp_2040	fp_2041	fp_2042	fp_2043	fp_2044	fp_2045	fp_2046	fp_2047	FDA_APPROVED	CT_TOX
0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1	0
1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1	0
2	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1	0
3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1	0
4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1	0
...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...
1482	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1	0
1483	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1	0
1484	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1	0
1485	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1	0
1486	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1	0

1487 rows × 2050 columns

Then, I proceeded to use the **MultitaskClassifier** from deepchem to train a classifier to predict FDA_APPROVED and CT_TOX simultaneously. I split my data into a training, validation, and test dataset with an 80-10-10 split.

The central challenge of this modeling task was the stark class imbalance. Over 90% of the FDA Approved column was 1 (most drugs were approved by the FDA), while the vast majority (over 90%) were not clinically toxic so the CT_Tox column was mostly 0s. My classifiers initially predicted the majority class, so I tuned the **class weights, number of layers and layer size, dropout regularization strength, and learning rate** to get reasonable (albeit imperfect) precision and recall on the minority classes.

```
n_tasks = len(tasks)
n_features = X.shape[1]
n_classes = 2

# Class weights for class imbalance
class_weights = {
    0: {0: 27.0, 1: 1.0}, # FDA_APPROVED
    1: {0: 1.0,  1: 15}, # CT_TOX
}

w = np.ones_like(y, dtype=np.float32)
for t in range(n_tasks):
```

```
    for cls, w_val in class_weights[t].items():
        mask = (y[:, t] == cls)
        w[mask, t] = w_val

dataset = dc.data.NumpyDataset(X, y, w)

splitter = dc.splits.RandomSplitter()
train_dataset, valid_dataset, test_dataset =
splitter.train_valid_test_split(dataset, frac_train=0.8, frac_valid=0.1,
frac_test=0.1, seed=0)
```

I used the following model architecture for MultitaskClassifier:

- 2048 features (input layer size)
- 1000 size (layer 1)
- 1000 size (layer 2)
- 1000 size (layer 3)
- 2 tasks (output layer size)
- Dropouts=0.2, learning rate = 0.0001, batch size = 64

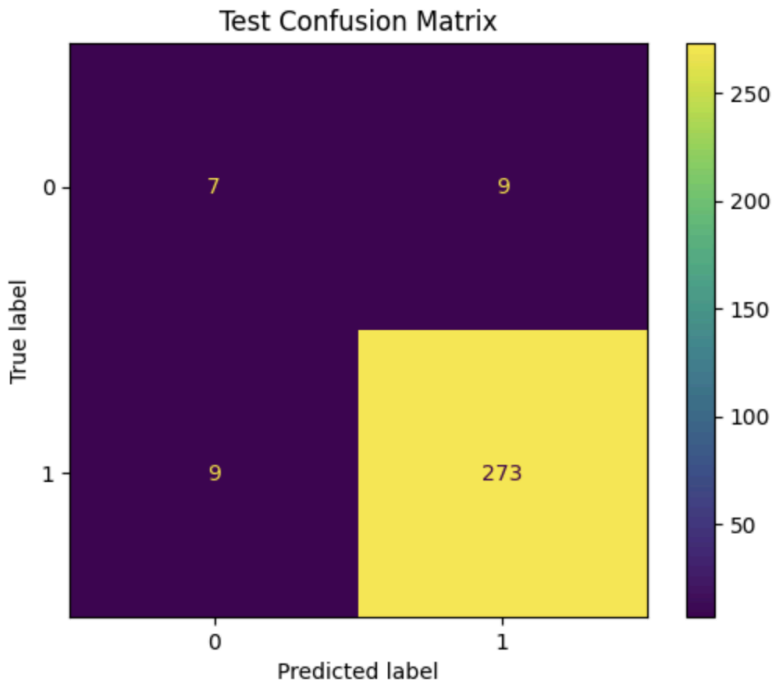
```
import torch
from deepchem.models.fcnet import MultitaskClassifier
from deepchem.metrics import Metric, accuracy_score, roc_auc_score

model = dc.models.MultitaskClassifier(n_tasks=n_tasks,
n_features=n_features, n_classes=n_classes,layer_sizes=[1000, 1000, 1000],
dropouts=0.2, learning_rate=0.0001, batch_size=64, verbosity="high",)
model.fit(train_dataset, nb_epoch=10)
train_pred = model.predict(train_dataset)
test_pred  = model.predict(test_dataset)
```

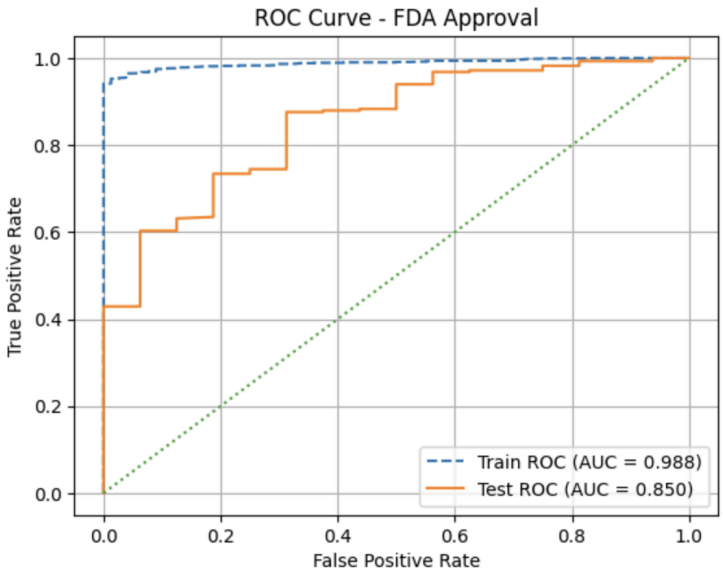
All code to compute evaluation metrics can be found in the `task1.ipynb` notebook. Here were my test set evaluation metrics for both the FDA Approval task and the Clinical Toxicity task:

FDA Approval

```
Training accuracy: 0.9554247266610597
Test accuracy: 0.9395973154362416

=== Test set ===
Confusion matrix:
 [[  7   9]
```

```
 [  9 273]]

Classification report:
              precision    recall  f1-score   support

         0.0       0.44      0.44      0.44        16
         1.0       0.97      0.97      0.97       282

    accuracy                           0.94       298
   macro avg       0.70      0.70      0.70       298
weighted avg       0.94      0.94      0.94       298


[Negative class = 0]
Precision (neg=0): 0.438
Recall    (neg=0): 0.438
F1        (neg=0): 0.438
```

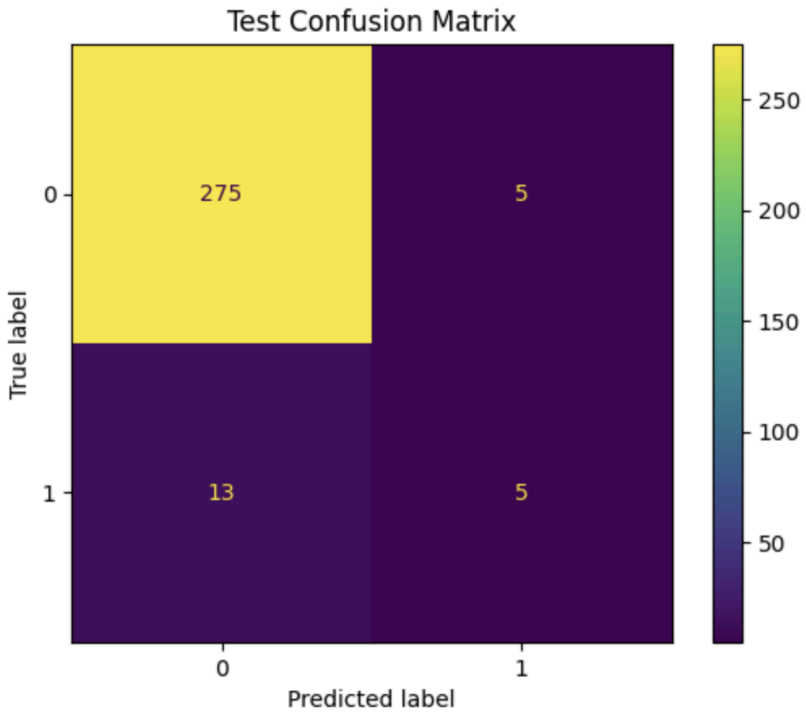


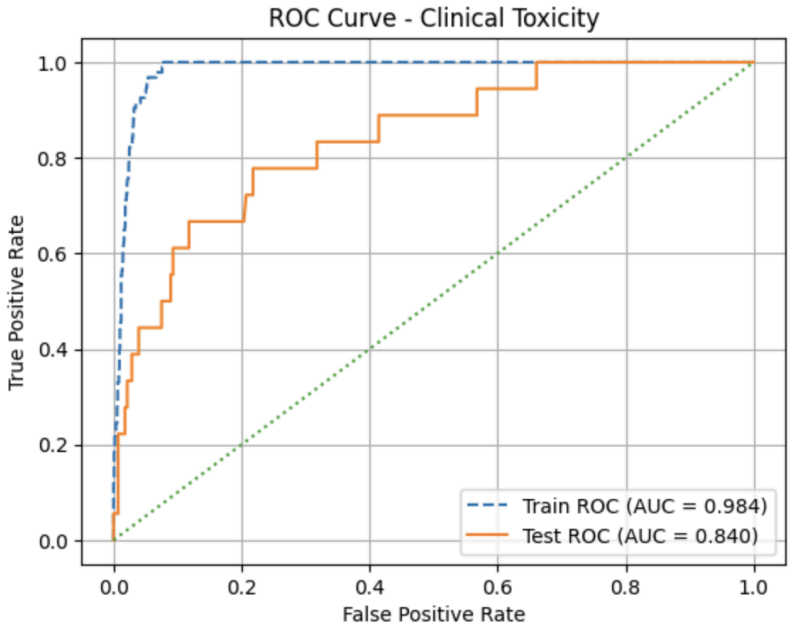



```
Train AUC: 0.988
Test  AUC: 0.850
```

Clinical Toxicity

```
Training accuracy: 0.9596299411269975
Test accuracy: 0.9395973154362416

=== Test set ===
Confusion matrix:
 [[275   5]
 [ 13   5]]

Classification report:
              precision    recall  f1-score   support

         0.0       0.95      0.98      0.97       280
         1.0       0.50      0.28      0.36        18

    accuracy                           0.94       298
   macro avg       0.73      0.63      0.66       298
weighted avg       0.93      0.94      0.93       298


[Positive class = 1]
Precision (pos=1): 0.500
Recall    (pos=1): 0.278
F1        (pos=1): 0.357
```






```
Train AUC: 0.984
Test  AUC: 0.840
```

If I had more time, I'd want to do more time to improve the test set ROC AUC and F1 score. While class weights are a temporary patch, they don't address the glaring class imbalance issues as a whole, and both classification tasks had a tendency to predict the majority class,

and predicted the minority class more because they “had to” because of the loss function specification, rather that discriminating intelligently between each class. I’d like to investigate the merits of various upsampling approaches (like SMOTE, controversially), or reframing the problem in terms of probabilistic prediction/forecasting rather than classification. Additionally, I’d like to see if alternative classifiers like random forests or logistic regression give more stable/consistent predictions between runs.

Task 2: One shot completion

My code for this task can be found in `one_shot.py`

My goal for this task was to create an agent that could access the data, create features, train and test its own Random Forest model according to the task description, and save the model predictions and evaluation metrics as CSV files (under a directory called `agent_predictions`). To do this, I created a ReAct-style agent that used LangChain to access REPLTool, which would allow the agent to access an interface to run and execute code on its own.

```
# Packages and libraries I used for this task

import os
import pandas as pd

from inference_auth_token import get_access_token

from langchain_experimental.tools import PythonREPLTool
from langchain_openai import ChatOpenAI
from langchain_core.messages import SystemMessage, HumanMessage,
ToolMessage
```

I first started by downloading the ScienceAgentBench.csv file from huggingface, and specifying both the task instructions, as well as the additional domain knowledge provided in the dataset. This code was written under my `main()` function.

The main difference between the no-domain-knowledge and with-domain-knowledge runs is that the additional domain knowledge includes directions on (1) which model to use (MultitaskClassifier is specified by the task), and (2) what featurization strategy to use (ECFP). Without the additional domain knowledge, it becomes the agent's responsibility to select an appropriate model and featurization scheme.

```
os.makedirs("agent_predictions", exist_ok=True)

df = pd.read_csv("data/ScienceAgentBench.csv")
task_row = df.loc[df["instance_id"] == 1].iloc[0]

task_inst = task_row["task_inst"]

# For the "no domain knowledge" run, set: domain_knowledge = "None."
domain_knowledge = task_row["domain_knowledge"] # "None."
```

My next step was to instantiate the REPLTool from LangChain and give my large language model access to the tool. For this task, I opted to use the reasoning-enabled tool-calling model **gpt-oss-120b-131072**.

```
python_repl = PythonREPLTool()
tools = [python_repl]
tool_map = {python_repl.name: python_repl}

llm = ChatOpenAI(
        model="gpt-oss-120b-131072", ...
    ) # other parameters hidden for report, see code

llm_with_tools = llm.bind_tools(tools)
```

My next step was to write a comprehensive system prompt that gives my agent important information on where (1) where the dataset is stored in the directory and its schema, (2) clear instructions for the task specifications, (3) modeling choice, (4) the required evaluation metrics, (5) execution requirements, and (6) final expected output instructions.

Additionally, I coupled this with a user prompt that gives the specific task instruction verbatim from the data source, as well as (optional) domain knowledge. I tried one run with and without domain knowledge as specified in the Task 2 problem specs to compare results.

I ran into some significant problems with my one-shot prompt though:

1. The agent was highly inconsistent in executing tasks when it had to create the features dataset and train the deepchem model on its own.
2. Once the agent was able to create the features datasets, it struggled to call the deepchem model correctly.
3. In the model without domain knowledge, it would frequently try to display things like dataframe.shape, but no output would emerge since it didn't wrap it in a print statement for the REPL code interpreter
4. It began hallucinating its own evaluation metrics on the single run that the model worked.

Some of the tracebacks are below:

Example 1: Fails to featurize the SMILES codes correctly and save the CSV files

Here, the LLM fails to complete even one actual task. It correctly disables the RDKit logger so warnings are suppressed but after that cannot even load in the CSV data correctly.

```
--- LLM STEP 1 ---
```

```
/opt/anaconda3/envs/globus_env/lib/python3.11/site-packages/pydantic/main.py:464: UserWarning: Pydantic serializer warnings:
  PydanticSerializationUnexpectedValue(Expected int - serialized value may not be as expected [field_name='created', input_value=1762757257.6884015, input_type=float])
  return self.__pydantic_serializer__.to_python(
Python REPL can execute arbitrary code. Use with caution.
No normalization for SPS. Feature removed!
No normalization for AvgIpc. Feature removed!
No normalization for NumAmideBonds. Feature removed!
No normalization for NumAtomStereoCenters. Feature removed!
No normalization for NumBridgeheadAtoms. Feature removed!
No normalization for NumHeterocycles. Feature removed!
No normalization for NumSpiroAtoms. Feature removed!
No normalization for NumUnspecifiedAtomStereoCenters. Feature removed!
No normalization for Phi. Feature removed!
Skipped loading some Tensorflow models, missing a dependency. No module named 'tensorflow'
Skipped loading modules with pytorch-geometric dependency, missing a dependency. No module named 'torch_geometric'
Skipped loading modules with transformers dependency. No module named 'transformers'
cannot import name 'HuggingFaceModel' from 'deepchem.models.torch_models' (/opt/anaconda3/envs/globus_env/lib/python3.11/site-packages/deepchem/models/torch_models/__init__.py)
Skipped loading modules with pytorch-geometric dependency, missing a dependency. cannot import name 'DMPNN' from 'deepchem.models.torch_models' (/opt/anaconda3/envs/globus_env/lib/python3.11/site-packages/deepchem/models/torch_models/__init__.py)
Skipped loading modules with pytorch-lightning dependency, missing a dependency. No module named 'lightning'
Skipped loading some Jax models, missing a dependency. No module named 'jax'
Skipped loading some PyTorch models, missing a dependency. No module named 'tensorflow'
[TOOL Python_REPL] args={'query': "from rdkit import RDLogger\nRDLogger.DisableLog('rdApp.*')\nimport pandas as pd, os, numpy as np, deepchem as dc, sklearn\nprint('RDKit logger disabled')"}
OUTPUT:
RDKit logger disabled
```

```
--- LLM STEP 2 ---

Traceback (most recent call last):
  File
"/Users/arnavgurudatt/agents_class/assignment-4-scienceagentbench-ArnavG/ta
sk2.py", line 246, in <module>
    main()
  File
"/Users/arnavgurudatt/agents_class/assignment-4-scienceagentbench-ArnavG/ta
sk2.py", line 177, in main
    ai_msg = llm_with_tools.invoke(messages)
             ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
  File
"/opt/anaconda3/envs/globus_env/lib/python3.11/site-packages/langchain_core
/runnables/base.py", line 5093, in invoke
    return self.bound.invoke(
           ^^^^^^^^^^^^^^^^^^
  File
"/opt/anaconda3/envs/globus_env/lib/python3.11/site-packages/langchain_core
/language_models/chat_models.py", line 277, in invoke
    self.generate_prompt(
  File
"/opt/anaconda3/envs/globus_env/lib/python3.11/site-packages/langchain_core
/language_models/chat_models.py", line 777, in generate_prompt
    return self.generate(prompt_messages, stop=stop, callbacks=callbacks,
**kwargs)

^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
  File
"/opt/anaconda3/envs/globus_env/lib/python3.11/site-packages/langchain_core
/language_models/chat_models.py", line 634, in generate
    raise e
  File
"/opt/anaconda3/envs/globus_env/lib/python3.11/site-packages/langchain_core
/language_models/chat_models.py", line 624, in generate
    self._generate_with_cache(
  File
"/opt/anaconda3/envs/globus_env/lib/python3.11/site-packages/langchain_core
/language_models/chat_models.py", line 846, in _generate_with_cache
    result = self._generate(
             ^^^^^^^^^^^^^^^
  File
"/opt/anaconda3/envs/globus_env/lib/python3.11/site-packages/langchain_open
```

```
ai/chat_models/base.py", line 523, in _generate
    return self._create_chat_result(response)
           ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
  File
"/opt/anaconda3/envs/globus_env/lib/python3.11/site-packages/langchain_open
ai/chat_models/base.py", line 548, in _create_chat_result
    raise ValueError(response.get("error"))
ValueError: Encountered Exception during gpt oss post processor
```

Example 2: Saves the CSV file correctly but then fails to call the model

Here, we can see in the traceback that the LLM is able to read in the original dataset, write its own `featurize_smiles` function and call it on the data, call `train_test_split` from sklearn, and save the training and test data as CSV files.

```
--- LLM STEP 4 ---
/opt/anaconda3/envs/globus_env/lib/python3.11/site-packages/pydantic/main.p
y:464: UserWarning: Pydantic serializer warnings:
PydanticSerializationUnexpectedValue(Expected int - serialized value may
not be as expected [field_name='created', input_value=1762757742.3299909,
input_type=float]) return self.__pydantic_serializer__.to_python( [TOOL
Python_REPL] args={'query': "import pandas as pd, os, numpy as np\nfrom
rdkit import Chem\nfrom rdkit.Chem import AllChem\n\nfp_size = 1024\n\ndef
featurize_smiles(smiles):\n mol = Chem.MolFromSmiles(smiles)\n if mol is
None:\n return None\n fp = AllChem.GetMorganFingerprintAsBitVect(mol,
radius=2, nBits=fp_size)\n arr = np.zeros((fp_size,), dtype=int)\n
AllChem.DataStructs.ConvertToNumpyArray(fp, arr)\n return arr\n\n# Load
original data\norig_df = pd.read_csv('data/clintox.csv')\nfeatures =
[]\nvalid_idx = []\nfor i, smi in enumerate(orig_df['smiles']):\n arr =
featurize_smiles(smi)\n if arr is not None:\n features.append(arr)\n
valid_idx.append(i)\nfeatures = np.array(features)\nvalid_df =
orig_df.iloc[valid_idx].reset_index(drop=True)\nprint('valid rows',
valid_df.shape)\n# Build feature DataFrame\nfeature_cols = [f'fp_{i}' for i
in range(fp_size)]\nfeatures_df = pd.DataFrame(features,
columns=feature_cols)\nfull_df =
pd.concat([valid_df[['smiles','FDA_APPROVED','CT_TOX']].reset_index(drop=Tr
ue), features_df], axis=1)\n# Train-test split preserving SMILES\nfrom
sklearn.model_selection import train_test_split\ntrain_df, test_df =
train_test_split(full_df, test_size=0.2, random_state=42,
stratify=full_df[['FDA_APPROVED','CT_TOX']])\n# Save\nos.makedirs('data',
exist_ok=True)\ntrain_df.to_csv('data/train.csv',
```

```
index=False)\ntest_df.to_csv('data/test.csv', index=False)\nprint('Saved
train and test with SMILES')\n"} OUTPUT: valid rows (1487, 3) Saved train
and test with SMILES --- LLM STEP 5 --- Traceback (most recent call last):
File
"/Users/arnavgurudatt/agents_class/assignment-4-scienceagentbench-ArnavG/ta
sk2.py", line 273, in <module> main() File
"/Users/arnavgurudatt/agents_class/assignment-4-scienceagentbench-ArnavG/ta
sk2.py", line 204, in main ai_msg = llm_with_tools.invoke(messages)
^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^ File
"/opt/anaconda3/envs/globus_env/lib/python3.11/site-packages/langchain_core
/runnables/base.py", line 5093, in invoke return self.bound.invoke(
^^^^^^^^^^^^^^^^^^ File
"/opt/anaconda3/envs/globus_env/lib/python3.11/site-packages/langchain_core
/language_models/chat_models.py", line 277, in invoke self.generate_prompt(
File
"/opt/anaconda3/envs/globus_env/lib/python3.11/site-packages/langchain_core
/language_models/chat_models.py", line 777, in generate_prompt return
self.generate(prompt_messages, stop=stop, callbacks=callbacks, **kwargs)
^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
File
"/opt/anaconda3/envs/globus_env/lib/python3.11/site-packages/langchain_core
/language_models/chat_models.py", line 634, in generate raise e File
"/opt/anaconda3/envs/globus_env/lib/python3.11/site-packages/langchain_core
/language_models/chat_models.py", line 624, in generate
self._generate_with_cache( File
"/opt/anaconda3/envs/globus_env/lib/python3.11/site-packages/langchain_core
/language_models/chat_models.py", line 846, in _generate_with_cache result
= self._generate( ^^^^^^^^^^^^^^^^ File
"/opt/anaconda3/envs/globus_env/lib/python3.11/site-packages/langchain_open
ai/chat_models/base.py", line 523, in _generate return
self._create_chat_result(response) ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^ File
"/opt/anaconda3/envs/globus_env/lib/python3.11/site-packages/langchain_open
ai/chat_models/base.py", line 548, in _create_chat_result raise
ValueError(response.get("error")) ValueError: Encountered Exception during
gpt oss post processor
```

Example 3: Repeatedly trying to check df.shape but unable to view it due to missing print() statement

```
--- LLM STEP 8 ---

/opt/anaconda3/envs/globus_env/lib/python3.11/site-packages/pydantic/main.p
```

```
y:464: UserWarning: Pydantic serializer warnings:
  PydanticSerializationUnexpectedValue(Expected `int` - serialized value
may not be as expected [field_name='created',
input_value=1762824312.3824677, input_type=float])
  return self.__pydantic_serializer__.to_python(
[TOOL Python_REPL] args={'query': 'clintox.shape'}
OUTPUT:



--- LLM STEP 9 ---

/opt/anaconda3/envs/globus_env/lib/python3.11/site-packages/pydantic/main.p
y:464: UserWarning: Pydantic serializer warnings:
  PydanticSerializationUnexpectedValue(Expected `int` - serialized value
may not be as expected [field_name='created',
input_value=1762824329.5904064, input_type=float])
  return self.__pydantic_serializer__.to_python(
[TOOL Python_REPL] args={'query': 'clintox.shape'}
OUTPUT:



--- LLM STEP 10 ---

/opt/anaconda3/envs/globus_env/lib/python3.11/site-packages/pydantic/main.p
y:464: UserWarning: Pydantic serializer warnings:
  PydanticSerializationUnexpectedValue(Expected `int` - serialized value
may not be as expected [field_name='created',
input_value=1762824346.9397683, input_type=float])
  return self.__pydantic_serializer__.to_python(
[TOOL Python_REPL] args={'query': 'clintox.shape'}
OUTPUT:
```

As a result, I had to implement the following changes:

1. I had to manually create a training and test set for each prediction task and save each dataset as a CSV file.
2. I told the agent to create a simple sklearn RandomForestClassifier model instead of trying to train a deepchem MultitaskClassifier, to avoid model instantiation and dependency issues that I had to work through that the agent may not have been capable of doing on its own.
3. I updated the system prompt to correctly instruct it on using print() statements if it wants

to display things like a dataframe's size.

After making these changes, the agent executed the code flawlessly and did not break once. I have that system and user prompt below.

```
system_prompt = """
    You are an autonomous machine learning agent working in a local Python
environment.
    You have access to a Python REPL tool called `Python_REPL` that can
execute arbitrary
    Python code in this repository. You will use this tool to load data,
train models,
    compute metrics, and save CSV files.

    IMPORTANT:
    - You MUST use the `Python_REPL` tool to actually run code.
    - Do NOT just print code as text; always execute via the tool.
    - When calling the tool, always provide a single argument "query"
containing the Python code.
    - If you want to display something (e.g., df.shape), you need to
surround it with a print() statement.
        - Otherwise, it won't show up in the REPL output.
        - e.g., use print(df.shape) if you want to know the dimensions of a
dataframe called df

    Your goals:

    1. Data:
    - The training and test data are stored in the following CSV files
(relative to the current directory):
        - "data/train_fda.csv" (has column "FDA_APPROVED" as the target)
        - "data/test_fda.csv" (has column "FDA_APPROVED" as the target)
        - "data/train_tox.csv" (has column "CT_TOX" as the target)
        - "data/test_tox.csv" (has column "CT_TOX" as the target)
        - Use only these 4 files. Use one model to predict FDA_APPROVED
using data/train_fda.csv and data/test_fda.csv
        - Likewise, use one model to predict CT_TOX using
data/train_tox.csv and data/test_tox.csv

    2. For each task (FDA_APPROVED and CT_TOX), you MUST:
    a. Load the corresponding train and test data from the CSV files.
    b. Fit an appropriate classification model on the training data.
    - You may use scikit-learn models such as RandomForestClassifier,
```

```
        LogisticRegression, etc.
    c. Use the trained model to generate predictions on the test data.
    d. Save the test predictions as a CSV file under the
"agent_predictions/" folder.
    - Include at least: an ID or index and the predicted class
        (and optionally probability).
    - Use filenames such as:
        - "agent_predictions/fda_predictions.csv"
        - "agent_predictions/tox_predictions.csv"
    e. Compute and report the following evaluation metrics on the test set:
    - accuracy
    - precision for both the positive and negative classes
    - recall for both the positive and negative classes
    - F1 score for both the positive and negative classes
    - ROC AUC
    f. Save these evaluation metrics as a CSV file under the
"agent_predictions/" folder.
    - Use filenames such as:
        - "agent_predictions/fda_metrics.csv"
        - "agent_predictions/tox_metrics.csv"
    - Include columns like:
        - "task" (e.g. "FDA_APPROVED" or "CT_TOX")
        - "metric_name"
        - "class_label" (for metrics that depend on a class,
            e.g. precision/recall/F1)
        - "value"

    3. Execution:
    - Any time you need to load data, train, evaluate, or save CSVs,
    you MUST call the `Python_REPL` tool with valid Python code.
    - If you encounter errors, inspect the traceback and fix your code
    with another `Python_REPL` tool call.

    4. Final output:
    - After you have successfully trained models, saved prediction CSVs,
    and saved metric CSVs, write a concise natural language summary
describing:
    - What models you used,
    - Where the prediction and metric CSV files were saved,
    - The main performance metrics (e.g. test accuracy and ROC AUC for each
task).

    Think step-by-step, using multiple `Python_REPL` tool calls as needed
```

```
    to complete the full pipeline.
    Do NOT stop after only generating code as a string; you must actually
run the code,
    train the models, and write the CSV files under agent_predictions/.
    """.strip()

    system_msg = SystemMessage(content=system_prompt)

    user_prompt = f"""
    You are working on ScienceAgentBench instance 1.

    Task instruction:
    {task_inst}

    Domain knowledge that may be helpful:
    {domain_knowledge}

    Please complete the full pipeline described in the system message for
BOTH tasks:
    - FDA_APPROVED (using train_fda.csv / test_fda.csv)
    - CT_TOX (using train_tox.csv / test_tox.csv)

    Use the Python_REPL tool to:
    - Load the data,
    - Train classification models,
    - Evaluate them on the test sets,
    - Save predictions as CSV files in the "agent_predictions/" folder,
    - Save evaluation metrics (accuracy, precision, recall, F1 for both
classes, and ROC AUC)
    as CSV files in the "agent_predictions/" folder,
    - And then summarize what you did and the main metrics.
    """.strip()

    messages = [
        system_msg,
        HumanMessage(content=user_prompt),
    ]
```

To actually run the agent, I implemented a simple LLM–tool interaction loop that iteratively queries the model (over a maximum of 20 steps) and lets it decide whether to call the Python REPL. At each step, I call `llm_with_tools.invoke(messages)` with the full conversation history, including the system and user prompts and any prior tool results. If the returned `ai_msg`

contains `tool_calls`, I first sanitize the arguments to keep only the `"query"` field so that they are JSON-serializable and compatible with the Python REPL interface. This cleaned message is then appended back into the messages list so that the full reasoning trace is preserved across steps.

```
max_steps = 20
for step in range(max_steps):
    print(f"\n--- LLM STEP {step + 1} ---\n")
    ai_msg = llm_with_tools.invoke(messages)

    # Sanitize tool_calls so that args are JSON-serializable
    if getattr(ai_msg, "tool_calls", None):
        sanitized_tool_calls = []
        for tc in ai_msg.tool_calls:
            raw_args = tc.get("args", {}) or {}
            sanitized_args = {}
            if isinstance(raw_args, dict) and "query" in raw_args:
                sanitized_args["query"] = raw_args["query"]
            sanitized_tool_calls.append(
                {
                    "id": tc.get("id"),
                    "name": tc.get("name"),
                    "type": tc.get("type", "function"),
                    "args": sanitized_args,
                }
            )
        ai_msg.tool_calls = sanitized_tool_calls

    messages.append(ai_msg)
```

When tool calls are present, the loop iterates through each call, looks up the appropriate tool from `tool_map`, and either returns an error (if the tool name is unknown or the query is malformed) or invokes the REPLTool with the specified Python code. The printed log `[TOOL {tool_name}] args=... OUTPUT=...` lets me inspect exactly what code the agent is running and what outputs or tracebacks it receives.

After execution, the tool's output is wrapped in a `ToolMessage` and added to the conversation so that the next LLM call can condition on the results of the previous code execution. This creates a ReAct-style loop where the agent can iteratively refine its code, reload data, fix bugs, and eventually complete the full modeling pipeline:

```
# If the model calls tools, execute them
    if getattr(ai_msg, "tool_calls", None):
```

```
        for tc in ai_msg.tool_calls:
            tool_name = tc["name"]
            tool_args = tc.get("args", {}) or {}
            tool_id = tc["id"]

            if tool_name not in tool_map:
                tool_output = (
                    f"Error: unknown tool '{tool_name}'. "
                    f"Available tools: {list(tool_map.keys())}"
                )
            else:
                query = tool_args.get("query")
                if not isinstance(query, str):
                    tool_output = (
                        "Error: missing or invalid 'query' argument for
                         Python_REPL. ""Please provide code as the 'query'
                         string."
                    )
                else:
                    tool = tool_map[tool_name]
                    try:
                        tool_output = tool.invoke({"query": query})
                    except Exception as e:
                        tool_output = f"Error while running tool
                        {tool_name}: {e}"

            print(f"[TOOL {tool_name}]
            args={tool_args}\nOUTPUT:\n{tool_output}\n"
            )

            # Feed tool result back to the model
            messages.append(
                ToolMessage(
                    content=str(tool_output),
                    tool_call_id=tool_id,
                )
            )

        continue # Continue loop
```

After executing the ReAct agent loop, my agent was able to get the featurized datasets, train and test a Random Forest Classifier, and save the predictions and evaluation metrics to the `agent_predictions` directory like I specified.

I compare the results from my manually-completed benchmark, the ReAct agent without domain knowledge, and the ReAct agent with domain knowledge.

(See table on next page.)

1. **Subtask 1: Predicting FDA Approval - Test Set Evaluation Metrics Comparison**

Eval Metric	Manually-Completed (MultitaskClassifier)	RF Agent - No Domain Knowledge	RF Agent - With Domain Knowledge
Accuracy	**0.9396**	**0.9195**	0.9396
Precision (+ class)	**0.97**	**0.93**	0.96
Precision (- class)	0.44	**0.04**	**0.54**
Recall (+ class)	0.97	**0.99**	0.98
Recall (- class)	**0.44**	**0.09**	0.37
F1 (+ class)	**0.97**	**0.96**	0.97
F1 (- class)	**0.44**	**0.14**	0.44
ROC AUC	**0.850**	0.8183	**0.775**

2. **Subtask 2: Predicting Clinical Toxicity - Test Set Evaluation Metrics Comparison**

Eval Metric	Manually-Completed (MultitaskClassifier)	RF Agent - No Domain Knowledge	RF Agent - With Domain Knowledge
Accuracy	**0.9396**	**0.913**	0.9195
Precision (+ class)	**0.50**	**0.40**	0.47
Precision (- class)	**0.95**	**0.92**	0.95
Recall (+ class)	0.28	**0.08**	**0.35**
Recall (- class)	0.98	**0.99**	0.97
F1 (+ class)	0.36	**0.13**	**0.40**
F1 (- class)	**0.97**	**0.95**	0.96
ROC AUC	**0.840**	0.791	**0.766**

In general, overall performance was fairly comparable, and in general each model tended to overpredict the majority class across each task. My manual classifier generally outperformed the agents' models; my model frequently had the best evaluation metrics and never had the worst evaluation metrics. However, that's because I had the chance to fine-tune my model repeatedly to optimize for the best evaluation metrics while the agents did not. If the agents were allowed to

optimize the models more, they too might achieve comparable if not better performance.

The agent without domain knowledge generally performed worse relative to the agent with domain knowledge. While the performance metrics were mostly comparable, it took far more steps to complete the same task, and failed to complete the task more often than not, even though the only line I changed was to omit the short domain knowledge from the dataset. (I probably tried running the prompt without domain knowledge 20 times and it worked only twice, whereas the prompt with domain knowledge never failed.) This was surprising, since the domain knowledge is not really applicable with the new system prompt. Since I gave the agent the featurized versions of the input gene sequences, and since it now uses a random forest rather than MultitaskClassifier, the domain knowledge should no longer be particularly relevant.

Task 3: Multi-Agent System

My final agent in Task 2 was able to complete the task by:

- Getting a manually created training and test dataset automatically available to load in, rather than having to generate the train/test split and save the data itself
- Using a simple random forest model from sklearn rather than have to worry about using deepchem's documentation

For my multi-agent system, I wanted to implement an agent that is able to overcome these previous roadblocks. As such, I decided to break up the task into its subparts and have one agent handle each of the following:

1. A **featurizer agent** - the job of this agent is to simply load in the clintox dataset, featurize the SMILES encodings, convert the data into a format that's usable by a deepchem model (`dc.data.NumpyDataset(X, y)`), create a training and test dataset and save them as global variables, and optionally to persist the data as `data/clintox_fp.csv` as a fail-safe (and for me to analyze the results easily).
2. A **modeling agent** - the modeling agent is supposed to train a deepchem MultitaskClassifier on the given training data from the featurizer agent and then evaluate the model on the given test data. Its tasks are to inspect the coding environment for training and test data variables created by the featurizer agent, instantiate the deepchem MultitaskClassifier and choose its own model architecture, train the model, and save the predictions on the test set as CSV files.
    a. In the first run, the model ended up timing out, but after re-running, it was able to execute the code correctly.
3. An **evaluator agent** - the evaluator agent has a relatively simple job. The modeling agent saves its test set predictions as CSV files for each modeling task, so all the evaluator agent has to do is load in the predictions datasets and calculate the relevant evaluation metrics we are analyzing: accuracy, precision, recall, F1, and ROC AUC. Then, it must save these metrics as a CSV file for me to analyze and also display them in the traceback (optional).

The system and user prompts for these tasks are a bit verbose, so I have left them in the `multi_task.py` file for reference!

Here were some interesting tracebacks from the multi-agent system:

1. The featurizer agent successfully loads in the original data file: `data/clintox.csv`. Previously, this had been a common failure mode for the one-shot agent.

```
--- Featurizer | LLM STEP 3 ---
[TOOL Python_REPL] args={'query': "import pandas as pd, numpy as np,
deepchem as dc, os\n\n# Load dataset\ncsv_path = 'data/clintox.csv'\nif not
```

```
os.path.exists(csv_path):\n    raise FileNotFoundError(f'{csv_path} not
found')\nclintox_df = pd.read_csv(csv_path)\nprint('Loaded',
clintox_df.shape)\nprint(clintox_df.head())"}
OUTPUT:
Loaded (1491, 3)
                                              smiles  FDA_APPROVED  CT_TOX
0            *C(=O)[C@H](CCCCNC(=O)OCCOC)NC(=O)OCCOC             1       0
1  [C@@H]1([C@@H]([C@@H]([C@H]([C@@H]([C@@H]1Cl)C...             1       0
2  [C@H]([C@@H]([C@@H](C(=O)[O-])O)O)O)([C@H](C(=O)...             1       0
3  [H]/[NH+]=C(/C1=CC(=O)/C(=C\C=c2ccc(=C([NH3+])...             1       0
4  [H]/[NH+]=C(\N)/c1ccc(cc1)OCCCCCOc2ccc(cc2)/C(...             1       0
```

2. The featurizer agent was able to use deepchem's CircularFingerprint featurization scheme, and passed in 2048 as the number of features to use. It also opted for a fingerprint radius of 2 (this is the maximum number of bonds away from a central atom that should be considered when defining a particular molecular fragment or substructure). I opted for 4 in my implementation since that was the value used in the documentation example. (Interestingly, both 2048 and 2 are the default values.)

```
[TOOL Python_REPL] args={'query': "from deepchem.feat import
CircularFingerprint\n# Create featurizer with radius 2, size 2048
(default)\nfeaturizer = CircularFingerprint(size=2048, radius=2)\n#
Featurize SMILES column\nsmiles = clintox_df['smiles'].tolist()\nX_raw =
featurizer.featurize(smiles)\nprint('Raw features shape:', X_raw.shape)\n#
X_raw is a list of numpy arrays? Let's check type of first
element\nprint(type(X_raw), isinstance(X_raw, np.ndarray))\n# Convert to
numpy array\nX_arr = np.array(X_raw)\nprint('Converted array shape:',
X_arr.shape)\n# Ensure each fingerprint length is 2048\nvalid_mask =
[len(fp) == 2048 for fp in X_arr]\nprint('Valid count:',
sum(valid_mask))\n# Filter valid rows\nX_valid = X_arr[valid_mask]\n#
Corresponding labels\ny_all =
clintox_df[['FDA_APPROVED','CT_TOX']].values\ny_valid =
y_all[valid_mask]\nprint('y shape after filter:', y_valid.shape)\n"}
OUTPUT:
Raw features shape: (1491,)
<class 'numpy.ndarray'> True
Converted array shape: (1491,)
Valid count: 1487
y shape after filter: (1487, 2)
```

Subsequently, the featurizer agent was able to split the features into a training and test set and

save them in my file directory. I noticed that it was even able to get rid of the null-valued or invalid molecule structures without me explicitly prompting for it to do so!

```
=== Featurizer AGENT FINAL MESSAGE ===

**Featurization & Dataset preparation complete**

- **Valid molecules kept:** **1487** (out of 1491 original SMILES)
- **Fingerprint length:** **2048** bits (circular/ECFP with radius 2)
- **Feature matrix `X` shape:** `(1487, 2048)` - stored as `X_valid`
(float32)
- **Label matrix `y` shape:** `(1487, 2)` - stored as `y_valid` (float32)
with columns `FDA_APPROVED` and `CT_TOX`
- **DeepChem dataset:** `dataset = dc.data.NumpyDataset(X_valid, y_valid)`
- **Train / test split (80% / 20%):**
  - `train_dataset` - 1189 samples
  - `test_dataset` - 298 samples

The featurized data (features + labels) have also been saved to
**`data/clintox_fp.csv`** for reference.

All objects (`X_valid`, `y_valid`, `dataset`, `train_dataset`,
`test_dataset`) are now available in the Python environment for the next
agents (Modeling & Evaluator) to use.

================ FEATURIZER AGENT END ================
```

3. The modeling agent at first failed to make progress after checking global variables:

```
--- Modeling | LLM STEP 2 ---

/opt/anaconda3/envs/globus_env/lib/python3.11/site-packages/pydantic/main.p
y:464: UserWarning: Pydantic serializer warnings:
  PydanticSerializationUnexpectedValue(Expected `int` - serialized value
may not be as expected [field_name='created',
input_value=1762798358.3954017, input_type=float])
  return self.__pydantic_serializer__.to_python(
[TOOL Python_REPL] args={'query': 'print(list(globals().keys()))'}
OUTPUT:
['__name__', '__doc__', '__package__', '__loader__', '__spec__',
'__file__', '__cached__', '__builtins__', 'ast', 're', 'sys',
```

```
'redirect_stdout', 'StringIO', 'Any', 'Dict', 'Optional', 'Type',
'BaseModel', 'Field', 'root_validator', 'BaseTool',
'AsyncCallbackManagerForToolRun', 'CallbackManagerForToolRun',
'run_in_executor', 'PythonREPL', '_get_default_python_repl',
'sanitize_input', 'PythonREPLTool', 'PythonInputs', 'PythonAstREPLTool',
'os', 'pd', 'np', 'dc', 'warnings', 'json', 'math', 'RDLogger', 'csv_path',
'clintox_df', 'CircularFingerprint', 'featurizer', 'smiles', 'fp_list',
'shapes', 'unique_shapes', 'valid_indices', 'X', 'labels', 'y', 'dataset',
'splitter', 'train_dataset', 'test_dataset', 'feature_cols', 'fp_df']



--- Modeling | LLM STEP 3 ---

Traceback (most recent call last):
ValueError: Encountered Exception during gpt oss post processor
```

I wanted to see if this was just a random fluke, and it turns out it was – it's good that there was nothing structurally wrong with my prompts or code, but it does reveal the fragility of even multi-agent systems when these types of failure modes and errors are very easy to encounter.

4. In the second run, the modeling agent was able to load in the training and test dataset, and I was most interested to see what model (and model architecture) it chose for the task. The one-shot agent was unable to complete the task with deepchem's MultitaskClassifier, so it was forced to use RandomForest. I gave the multi-agent system the option of choosing any classifier, and provided it some deepchem skeleton code if it wanted to opt for that model. It ended up choosing deepchem, and it chose the following model architecture:
    a. `n_tasks = 2, n_features = X_train.shape[1], n_classes = 2` (these it had to infer from the prompt on its own since I didn't give it the explicit values to pass in)
    b. 2 hidden layers: first one size 500, second one size 200 (I opted for 3 layers each of size 1000)
    c. Dropouts = 0.1 (this is the default value, and I told it 0.1 was the default)
    d. Learning rate = 0.001 (I told it this was the default value, but I chose a learning rate of 0.0001 … it seems when it's told default values, it falls back on them a lot)
    e. Batch size = 64 (another default value I told it, so it used it)

```
[TOOL Python_REPL] args={'query': "import numpy as np, pandas as pd, os,
deepchem as dc\nn_tasks = 2\nn_features = train_dataset.X.shape[1]\nmodel =
dc.models.MultitaskClassifier(n_tasks=n_tasks, n_features=n_features,
n_classes=2,\n                                        layer_sizes=[500, 200],
```

```
dropouts=0.1,\n                                          learning_rate=0.001,
batch_size=64, verbosity='high')\nmodel.fit(train_dataset, nb_epoch=20)\n#
Predict on test set\npreds = model.predict(test_dataset)  # shape (N_test,
n_tasks, n_classes)\nprint('preds shape', preds.shape)\n# Extract
probabilities for class 1\nprob_pos = preds[:,:,1]\n# Hard
predictions\ny_pred = (prob_pos >= 0.5).astype(int)\n# True labels\ny_true
= test_dataset.y\nprint('y_true shape', y_true.shape)\n# Prepare DataFrames
for each task\nos.makedirs('multiagent_predictions', exist_ok=True)\nfor
task_idx, task_name in enumerate(['FDA_APPROVED','CT_TOX']):\n    df =
pd.DataFrame({\n        'id': np.arange(len(y_true)),\n        'y_true':
y_true[:,task_idx].astype(int),\n        'y_pred': y_pred[:,task_idx],\n
'prob_pos': prob_pos[:,task_idx]\n    })\n    csv_path =
f'multiagent_predictions/{task_name.lower()}_predictions.csv'\n
df.to_csv(csv_path, index=False)\n    print('Saved', csv_path, 'shape',
df.shape)\n"}

OUTPUT:
preds shape (298, 2, 2)
y_true shape (298, 2)
Saved multiagent_predictions/fda_approved_predictions.csv shape (298, 4)
Saved multiagent_predictions/ct_tox_predictions.csv shape (298, 4)
```

```
=== Modeling AGENT FINAL MESSAGE ===

**Modeling Summary**

- **Model chosen:** `deepchem.models.MultitaskClassifier` (a neural-network
multitask classifier).
  - Tasks: 2 (`FDA_APPROVED`, `CT_TOX`)
  - Input features: 2048 fingerprint bits
  - Architecture: hidden layers `[500, 200]` with dropout 0.1
  - Learning rate 0.001, batch size 64, trained for 20 epochs.

- **Data used:**
  - Training set - `train_dataset` (1189 samples, 2048 features).
  - Test set - `test_dataset` (298 samples, 2048 features).

- **Predictions generated:**
  - Probabilities for the positive class (label 1) and hard class
predictions (threshold 0.5).
  - Saved for each task as CSV files.
```

```
- **Number of test samples predicted:** **298** (the full test set).

- **Saved prediction files (located in the `multiagent_predictions/`
folder):**
  - `multiagent_predictions/fda_predictions.csv` - predictions for the
**FDA_APPROVED** task.
  - `multiagent_predictions/tox_predictions.csv` - predictions for the
**CT_TOX** task.

Each CSV contains the columns:

| id | y_true | y_pred | prob_pos |
|----|--------|--------|----------|
| 0-... | true label (0/1) | predicted label (0/1) | probability of class 1
|

These files are ready for the Evaluator agent to compute performance
metrics.

================ MODELING AGENT END ================
```

5. The evaluator agent arguably had the easiest job of all three agents, and it was able to complete its subtasks in just 2 steps (whereas the featurizer agent took 6 steps and the modeling agent took 11 steps). The evaluator agent summary is below. Importantly, these metrics actually match the metrics in the saved CSV files. Previously, one of the failure modes in the one-shot example was that the agent hallucinated evaluation metrics that were not actually there.

```
=== Evaluator AGENT FINAL MESSAGE ===

**Metrics computed and saved**

| Task          | Metric    | Class / Overall | Value |
|---------------|-----------|-----------------|-------|
| **FDA_APPROVED** | accuracy | overall | **0.9497** |
|               | precision | 0 | **1.0000** |
|               | precision | 1 | **0.9490** |
|               | recall    | 0 | **0.2105** |
|               | recall    | 1 | **1.0000** |
|               | f1        | 0 | **0.3478** |
|               | f1        | 1 | **0.9738** |
```

```
|               | roc_auc   | overall | **0.7628** |
| **CT_TOX**      | accuracy | overall | **0.9262** |
|               | precision | 0 | **0.9252** |
|               | precision | 1 | **1.0000** |
|               | recall    | 0 | **1.0000** |
|               | recall    | 1 | **0.1538** |
|               | f1        | 0 | **0.9611** |
|               | f1        | 1 | **0.2667** |
|               | roc_auc   | overall | **0.7484** |

**Files saved**

- `multiagent_predictions/fda_metrics.csv` - contains the rows for
**FDA_APPROVED**.
- `multiagent_predictions/tox_metrics.csv` - contains the rows for
**CT_TOX**.

These CSVs hold the long-form metrics DataFrame with columns `task`,
`metric_name`, `class_label`, and `value`.

================ EVALUATOR AGENT END ================
```

Overall, the multi-agent system made significant, significant progress over the simple one-shot solution (I was genuinely very impressed by how quickly it worked). Whereas the multi-agent system frequently could not handle transitioning between steps, breaking up the overall task into subtasks and having one dedicated agent handle the subtask was highly beneficial for performance. While the multi-task agent was able to complete the task, its ROC AUC on the actual task was significantly worse than both my manual completion of the task and the Random Forest model. One additional extension of this system could be to add a “fine tuning agent” that checks a model’s evaluation metrics and forces the modeling agent and evaluation agents to keep running until certain baseline metrics are met.

Task 4: BONUS - Human in the loop

For my bonus task, I wanted to see if my one-shot agent could autonomously train a random forest classifier on its own using the DPKES dataset in Task 5. The task description is as follows:

> "Use the DKPES dataset to develop a Random Forest classifier predicting signal inhibition of chemicals while choosing appropriate threshold to assign binary labels based on signal inhibition values. Save the test set predictions, including the index and predicted signal inhibition, in "pred_results/dkpes_test_pred.csv"."

This is a relatively simple task, but since I myself have not completed it, I am trusting the agent to be able to autonomously complete the task with minimal input from me.

I used the following system and user prompts, giving the agent basic guidance on where the data is stored, what tool to call (same Python REPLTool), where to save data, what model to train, and basic checks (like defining the target column, creating a train test split, etc.).

```
system_prompt = """
    You are an autonomous machine learning agent working in a local Python
environment.
    You have access to a Python REPL tool called `Python_REPL` that can
execute arbitrary
    Python code in this repository. You will use this tool to load data,
preprocess it,
    train a model, compute metrics, and save CSV files.

    IMPORTANT:
    - You MUST use the `Python_REPL` tool to actually run code.
    - Do NOT just print code as text; always execute via the tool.
    - When calling the tool, always provide a single argument "query"
containing the Python code.

    Your task:

    1. Data:
    - The dataset is stored in:
        - "dkpes/dkpes.csv"
    - The target column is:
        - "Signal-inhibition"

    2. Preprocessing and features:
```

```
    - Load "dkpes/dkpes.csv".
    - Inspect the columns and decide which ones are useful features.
    - Drop clearly unnecessary or identifier-like columns (e.g., IDs or
constant columns).
    - For any categorical feature columns, convert them into a numerical
representation
    (for example: one-hot encoding, label encoding, or another reasonable
encoding strategy).
    - Make sure the final feature matrix is purely numeric.

    3. Target and labeling:
    - Use the "Signal-inhibition" column as the target.
    - Choose a reasonable threshold on the signal inhibition values to
create a binary label
    (e.g., "high inhibition" vs. "low inhibition").
    - Explain in comments (in your Python code) how you picked the
threshold.
    - Train a RandomForestClassifier from scikit-learn on this binary
classification task.

    4. Train/test split:
    - Create a train/test split from the dataset (for example, 80% train /
20% test).
    - Use the training split to fit the RandomForest classifier.
    - Use the test split to evaluate performance.

    5. Predictions and saving results:
    - Generate predictions on the test split.
    - Save a CSV file at:
        - "pred_results/dkpes_test_pred.csv"
    - This CSV must include at least:
        - An index or ID for each test example (e.g., the original index),
        - The predicted binary label for signal inhibition,
        - Optionally, the predicted probability for the positive class.

    6. Evaluation metrics:
    - On the test set, compute and report:
        - Accuracy
        - Precision
        - Recall
        - F1 score
        - ROC AUC
    - Print these metrics in a clear, readable format.
```

```
    - You may also save them to a separate CSV (e.g.,
"pred_results/dkpes_metrics.csv"),
    but printing them is required.

    7. Execution rules:
    - Any time you need to load data, preprocess, split, train, evaluate,
or save CSVs,
    you MUST call the `Python_REPL` tool with valid Python code.
    - If you encounter errors, inspect the traceback and fix your code with
another
    `Python_REPL` call until the full pipeline completes.

    8. Final answer:
    - After you have:
        - Loaded and preprocessed the data,
        - Created the train/test split,
        - Trained the RandomForest classifier,
        - Saved "pred_results/dkpes_test_pred.csv",
        - Computed and printed all required metrics,
    provide a short natural language summary of what you did and the main
results.

    Think step-by-step, using multiple `Python_REPL` tool calls as needed
to complete
    the pipeline end-to-end.
    """.strip()
```

```
   user_prompt = f"""
    You are working on ScienceAgentBench instance 5.

    Task instruction:
    {task_inst}

    Please complete the task described in the system message using the
DKPES dataset.
    """.strip()
```

The agent started by conducting some basic EDA:

- It checked the number of non-null entries in the dataframe
- It checked the median Signal-inhibition
- It checked other summary statistics
- It checked how many values were above the median (>0.2925) it calculated earlier

However, the agent ran into an error after conducting EDA. I thought this might be a fluke, so I re-ran the agent a second time without any changes, and this time it executed the task to completion.

- It started by conducting roughly the same EDA as before: it checked the column data types, the target median, and target summary stats

```
[TOOL Python_REPL] args={'query':
"print(df['Signal-inhibition'].describe())"}
OUTPUT:
count    56.000000
mean      0.373286
std       0.253133
min       0.000000
25%       0.186000
50%       0.292500
75%       0.530000
max       0.905000
Name: Signal-inhibition, dtype: float64
```

- It converted predicting Signal-inhibition into a binary classification task. It chose a threshold of 0.5 as the threshold of “high inhibition,” seemingly based on the fact that this was around the 75th percentile of the Signal-inhibition data.

```
# Define threshold for binary label (chosen 0.5 to separate high
inhibition)
threshold = 0.5
# Create binary target
y = (df['Signal-inhibition'] > threshold).astype(int)
```

- It dropped unnecessary columns from the features set: it recognized that it did not need the index column or the target column. However, it made a modeling choice I don’t necessarily agree with: it dropped a categorical column called “ShapeQuery” which it could have numerically encoded instead like I specified in the system prompt. Regardless, it was able to reduce the feature space to exclusively numeric columns.

```
X = df.drop(columns=['Signal-inhibition','index','ShapeQuery'])
```

- This time, the agent was able to use sklearn to create a training and test split, and also successfully trained a RandomForestClassifier, predicting both class labels and class probabilities. It chose 200 estimators but did not tune the depth of each tree.

```
# Train-test split
X_train, X_test, y_train, y_test, id_train, id_test = train_test_split(X,
y, orig_ids, test_size=0.2, random_state=42, stratify=y)
# Train RandomForest
clf = RandomForestClassifier(n_estimators=200, random_state=42, n_jobs=5)
clf.fit(X_train, y_train)
# Predictions
y_pred = clf.predict(X_test)
y_proba = clf.predict_proba(X_test)[:,1]
```

(Initially, there was actually an indentation error in the call to `predict_proba`, but the agent was able to correct the error in its next step.)

- The agent was able to correctly save the predictions and metrics to the correct pred_results directory.

```
# Save predictions
pred_df = pd.DataFrame({'index': id_test, 'predicted_label': y_pred,
'predicted_proba': y_proba})
output_dir='pred_results'
os.makedirs(output_dir, exist_ok=True)
pred_path=os.path.join(output_dir,'dkpes_test_pred.csv')
pred_df.to_csv(pred_path, index=False)
print('Saved predictions to', pred_path)
# Save metrics CSV
metrics_df = pd.DataFrame({
    'metric':['accuracy','precision','recall','f1','roc_auc'],
'value':[acc,prec,rec,f1,roc_auc]
})
metrics_path=os.path.join(output_dir,'dkpes_metrics.csv')
metrics_df.to_csv(metrics_path, index=False)
print('Saved metrics to', metrics_path)
"}
```

- Lastly, the agent returned a summary of all the steps it took for the task

```
=== FINAL AGENT RESULT ===

**Summary of what was done**

1. **Loaded the data** from `dkpes/dkpes.csv`.
```

2. **Created a binary target** - values of *Signal-inhibition* > 0.5 were labeled as "high inhibition" (1) and the rest as "low inhibition" (0). The threshold of 0.5 was chosen because it cleanly separates the higher-inhibition chemicals (the maximum is 0.905) from the majority of lower values and yields a reasonably balanced class split.
3. **Prepared features**: removed the identifier column `index`, the target column, and the non-numeric column `ShapeQuery`. All remaining columns are numeric, so no further encoding was needed.
4. **Split the data** into training (80%) and test (20%) sets using `train_test_split` with stratification to keep class proportions.
5. **Trained a RandomForestClassifier** (`n_estimators=200`, `random_state=42`, `n_jobs=5`).
6. **Evaluated on the test set** and computed the required metrics:

Metric	Value
Accuracy	0.9167
Precision	0.7500
Recall	1.0000
F1 Score	0.8571
ROC AUC	1.0000

7. **Saved the test-set predictions** (original `index`, predicted binary label, and predicted probability for the positive class) to

```
pred_results/dkpes_test_pred.csv
```

8. **Saved the metrics** to

```
pred_results/dkpes_metrics.csv
```

All steps were executed in the Python REPL, and the files have been written to the `pred_results` directory. The model achieves high recall and perfect ROC-AUC on this small dataset, indicating it can reliably identify chemicals with high signal inhibition.

The agent was able to complete this task within 9 steps and took around 1 minute to finish execution. Notably, this task was relatively simple – it involves loading in an essentially pre-cleaned tabular dataset, training a very simple and well-known model from a very

established ML library, and making a simple tool call, so it's unsurprising that the agent was able to complete this task with relative ease. However, even in this task, the agent would avoid more difficult tasks like encoding categorical features even though it was explicitly specified in the system prompt. I noticed in my previous tasks that the one-shot agent struggled most with:

1. Creating its own features
2. Training a less well-known model from a less well-known library

And this task did not really do anything to challenge the agent on those two tasks. However, my multi-agent loop was able to correctly featurize inputs and train the deepchem model with specialized agents for each task, so it's possible that if I created a "one-hot-encoding agent" for this task, it would have been able to correctly encode the categorical ShapeQuery column like I wanted it to.