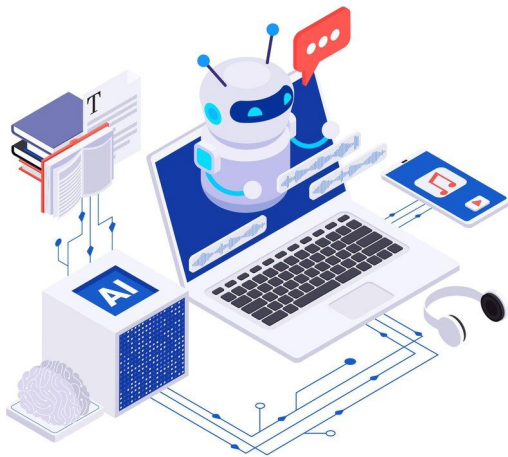


Enhancing Operational Data Synthesis and Predictive Analysis in HPC Clusters Using Large Language Models



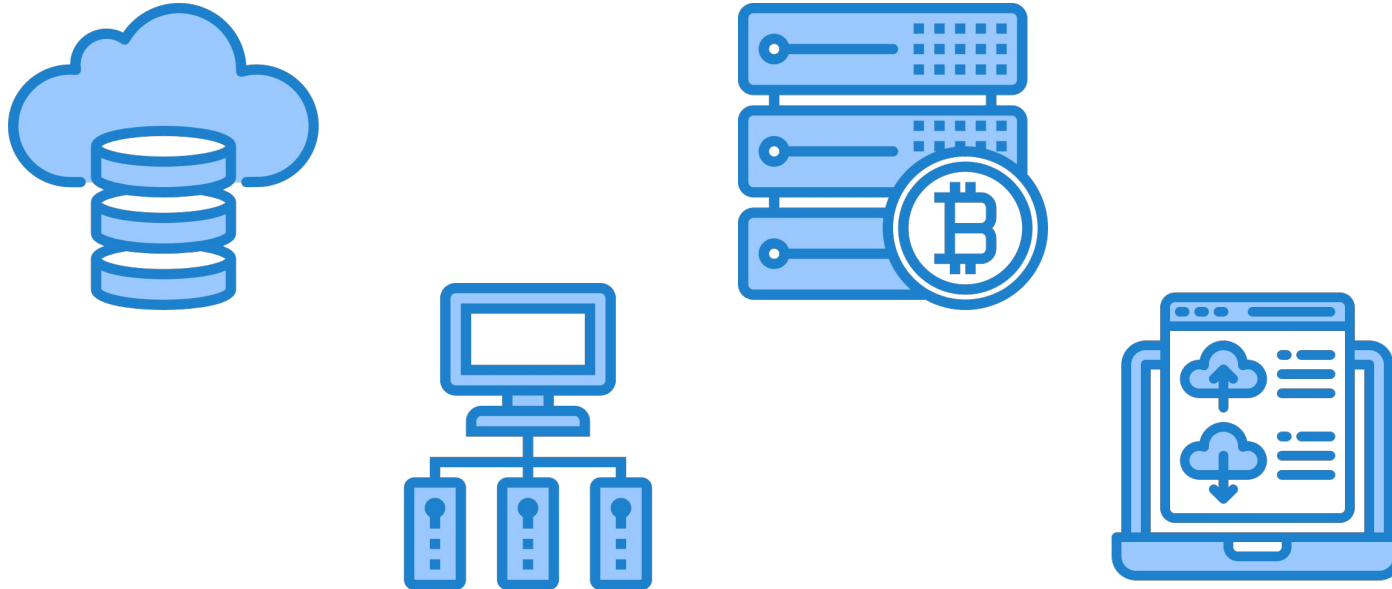
Source: freepik.com

Yizhen Zang

Daily Supervisor: Xiaoyu Chu

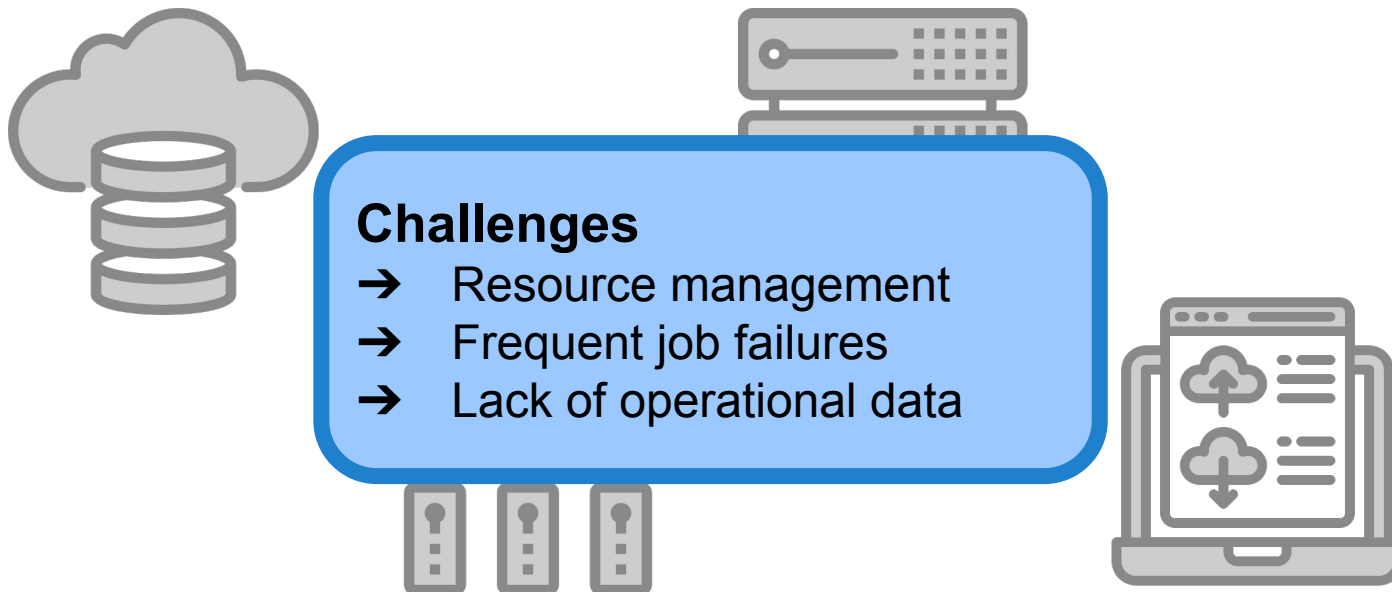
July, 2024

HPC Clusters are Vital to Digital Society



Source: flaticon.com

HPC Clusters are Vital to Digital Society



Source: flaticon.com

HPC Clusters are Vital to Digital Society

Impact of HPC Outages

- **Prevalence:** 80% of users
- **Cost:** 60% resulted in at least **\$100,000** losses

Source: Uptime Institute, Annual outages analysis 2023

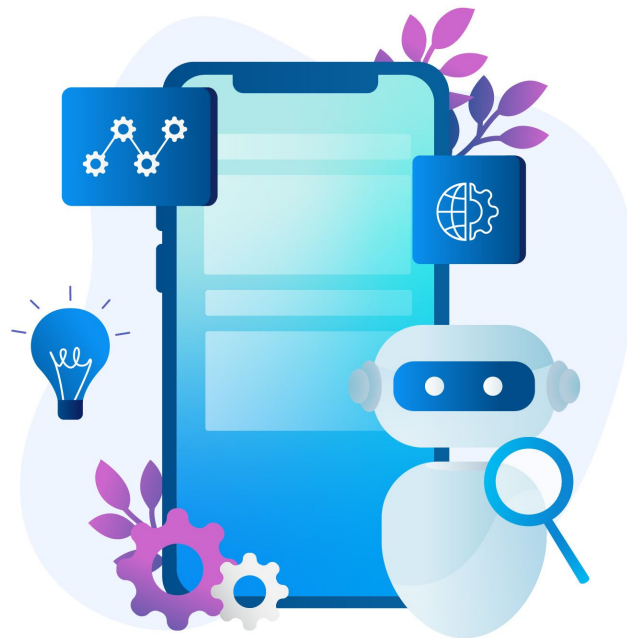


Source: freepik.com

Large Language Models are Powerful

Traditional Models

- Limited Adaptability
- Simplistic Approaches
- Inflexibility



Source: freepik.com

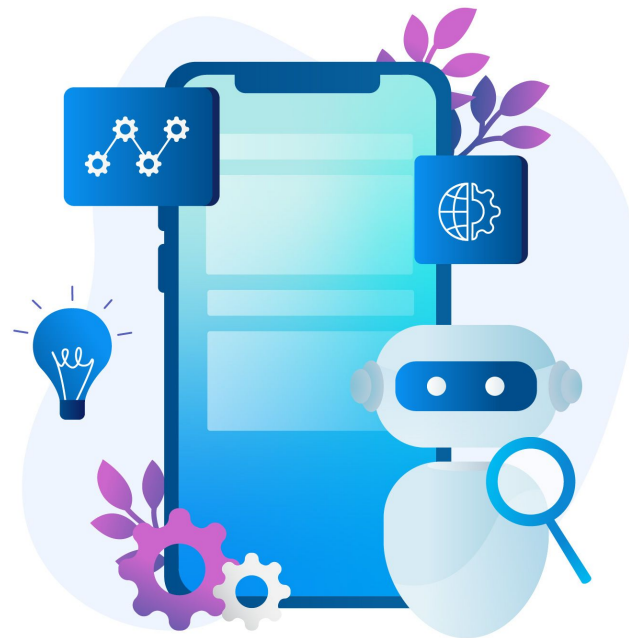
Large Language Models are Powerful

Traditional Models

- Limited Adaptability
- Simplistic Approaches
- Inflexibility

LLMs

- ★ High Adaptability
- ★ Complex Data Handling
- ★ Flexibility and Integration



Source: freepik.com

Research Questions

The overarching RQ: How to leverage LLMs to improve operational decision-making for HPC datacenters?

Research Questions

RQ1: What are the existing applications of LLMs for HPC?

RQ1.1: How are LLMs applied in HPC for **workload synthesis**?

RQ1.2: How are LLMs applied in HPC for **workload prediction**?

RQ1.3: How are LLMs applied in **other tasks** in HPC?

Research Questions

RQ1: What are the existing applications of LLMs for HPC?

RQ2: How to design and evaluate LLM-based models for synthesizing job data in HPC clusters?

RQ2.1: How to generate synthetic job data in HPC clusters using LLMs?

RQ2.2: How are the techniques developed in **RQ2.1** performing, relative to the non-LLM state-of-the-art?

Research Questions

RQ1: What are the existing applications of LLMs for HPC?

RQ2: How to design and evaluate LLM-based models for synthesizing job data in HPC clusters?

RQ3: How to design and evaluate LLM-based models for predicting job end-state in HPC clusters?

RQ3.1: How to predict job failures in HPC clusters using LLMs?

RQ3.2: How are the techniques developed in **RQ3.1** performing, relative to the non-LLM state-of-the-art?

Literature Review of LLMs Applications in HPC

RQ1

Reference	Applications	Models	Datasets
Shi et al.	memory workload synthesis	REaLTabFormer	SPEC2017
LM4HPC	code similarity analysis parallelism detection OpenMP Q&A	CodeBERT GraphCodeBERT gpt-3.5-turbo	POJ-104 DRB-ML OMP4Par OMPQA
MPiIrigen	MPI-based parallel program	MonoCoder PolyCoder GPT-3.5	HPCorpusMPI
HPC-Coder	code completion OpenMP labeling performance prediction	GPT-2 GPT-Neo PolyCoder	self-collected
HPC-GPT	AI model management dataset management data race detection	LLaMa LLaMa 2	self-collected
LLMDB	query rewrite database diagnosis data analytics	LLMDB	self-collected

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Workload synthesis

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Workload synthesis

Code-based tasks

Literature Review of LLMs Applications in HPC

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Workload synthesis

Code-based tasks

Data management

Literature Review of LLMs Applications in HPC

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LM4HPC	code similarity analysis parallelism detection OpenMP Q&A	CodeBERT GraphCodeBERT gpt-3.5-turbo	POJ-104 DRB-ML OMP4Par OMPQA		
MP	<div>Gaps remain in workload synthesis and prediction.</div>				
HP					
	performance prediction	PolyCoder			
HPC-GPT	AI model management dataset management data race detection	LLaMa LLaMa 2	self-collected	Data management	
LLMDB	query rewrite database diagnosis data analytics	LLMDB	self-collected		

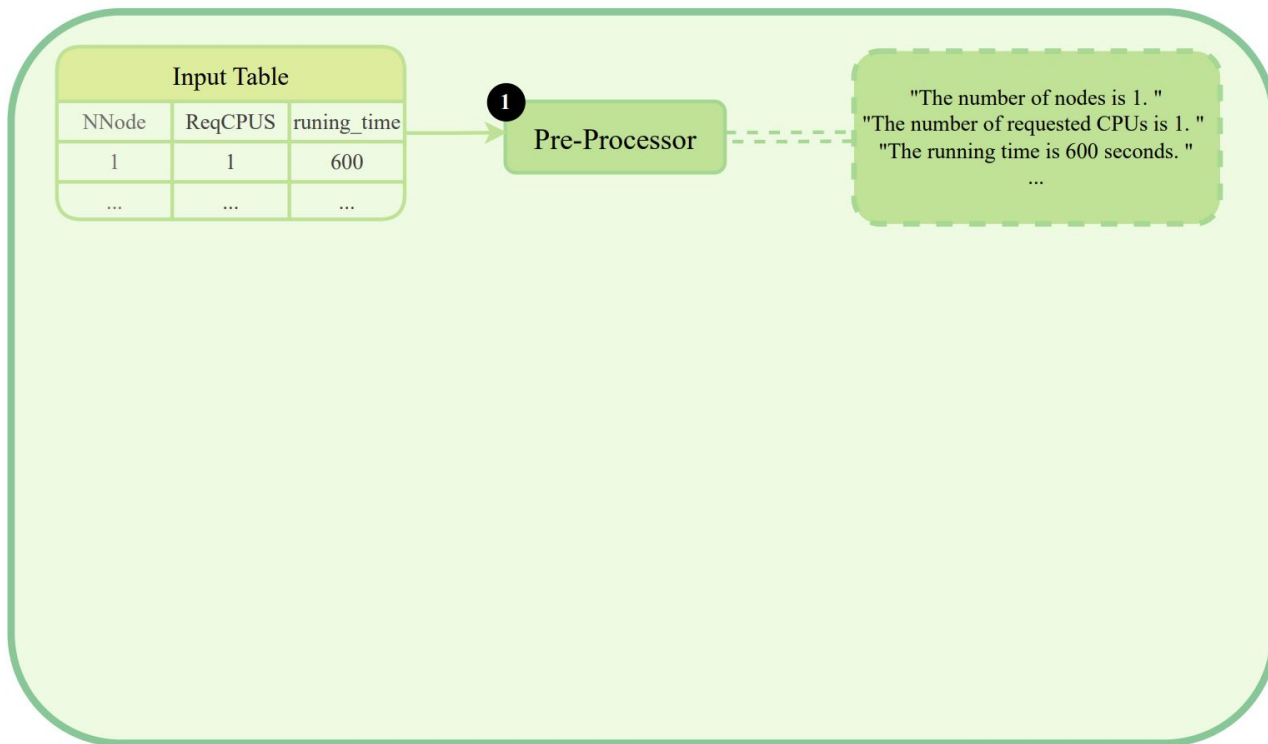
Design - How to Use LLMs for Job Data Synthesis?

RQ2.1

Input Table		
NNode	ReqCPUS	runing_time
1	1	600
...

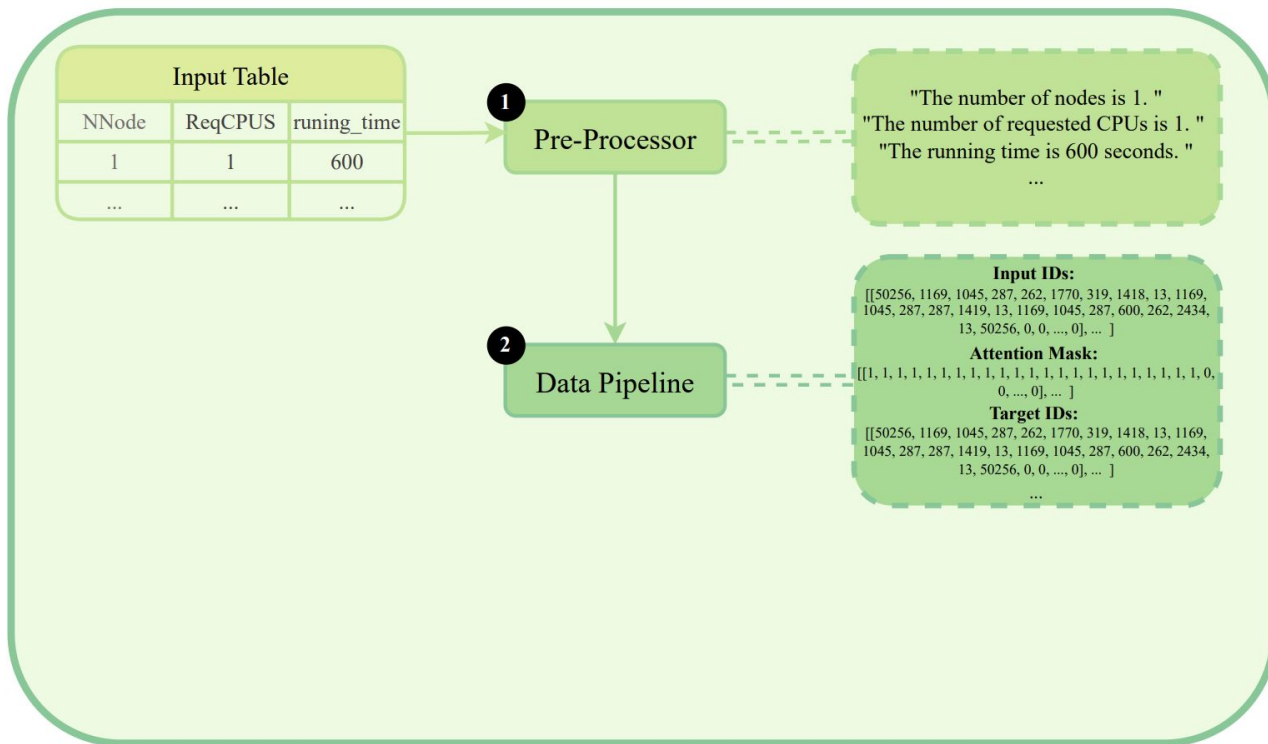
Design - How to Use LLMs for Job Data Synthesis?

RQ2.1



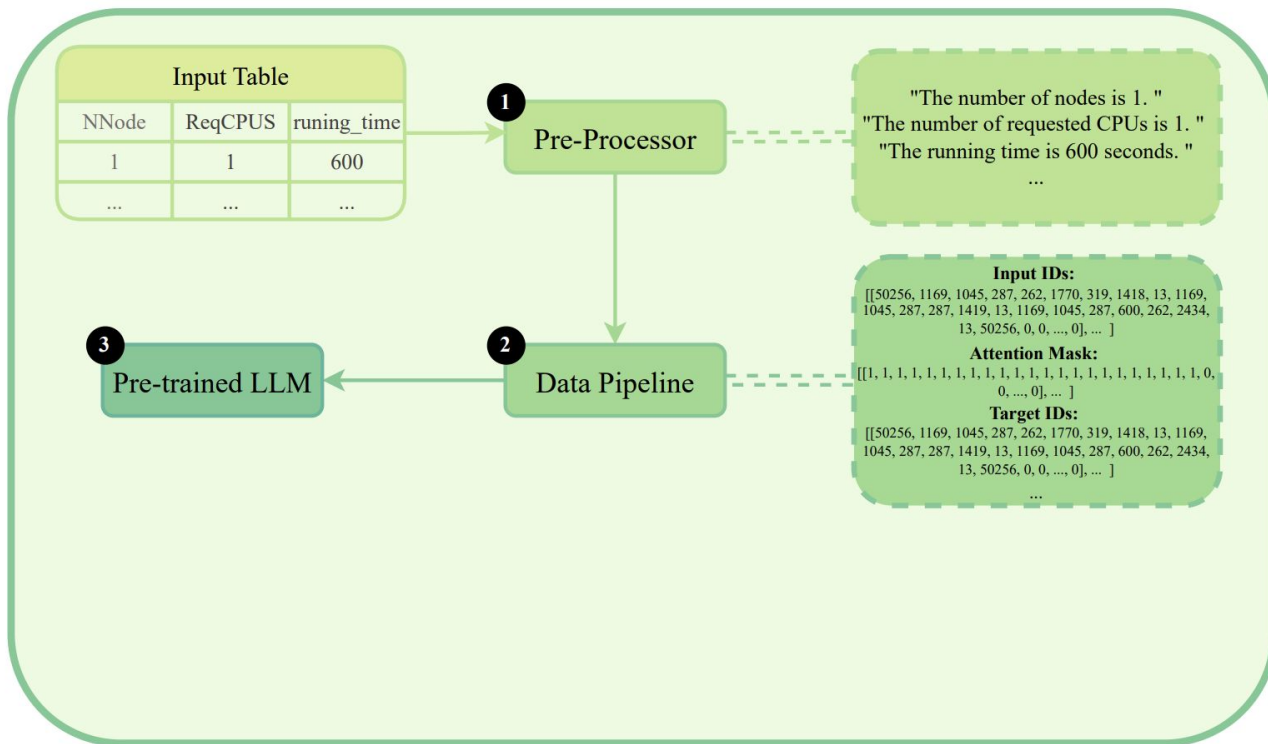
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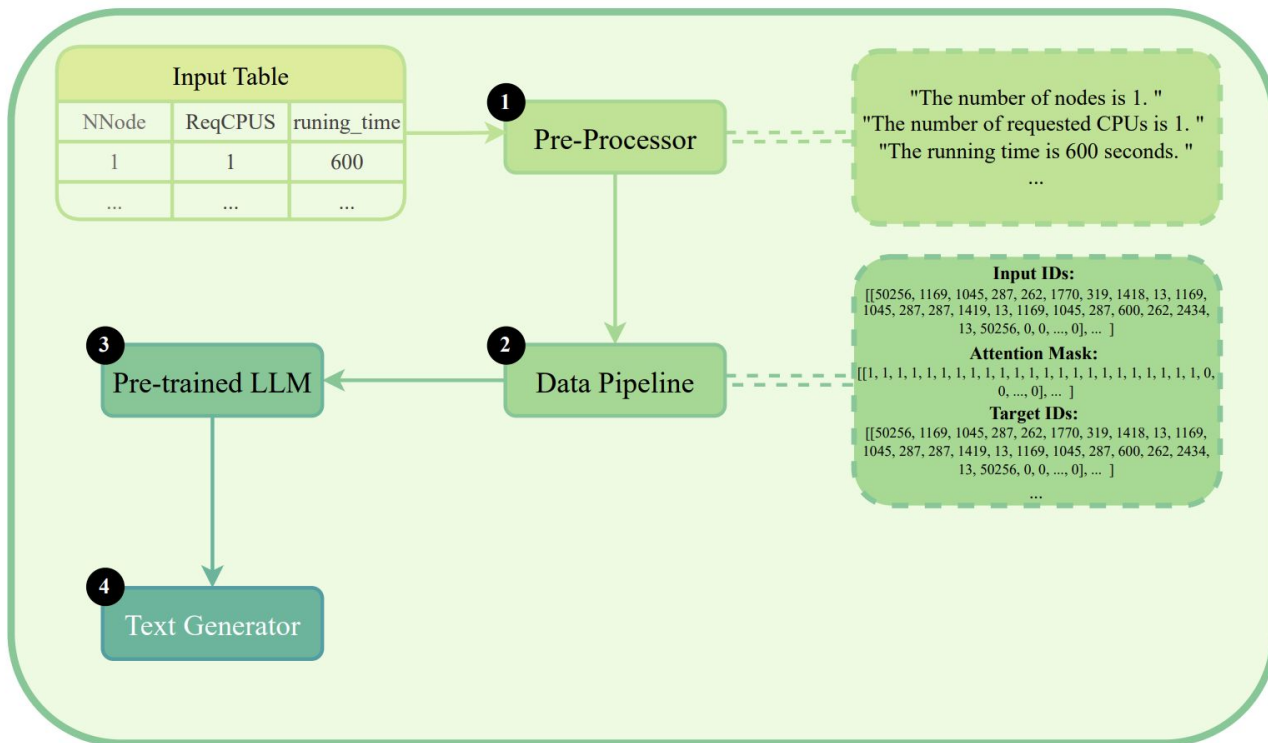
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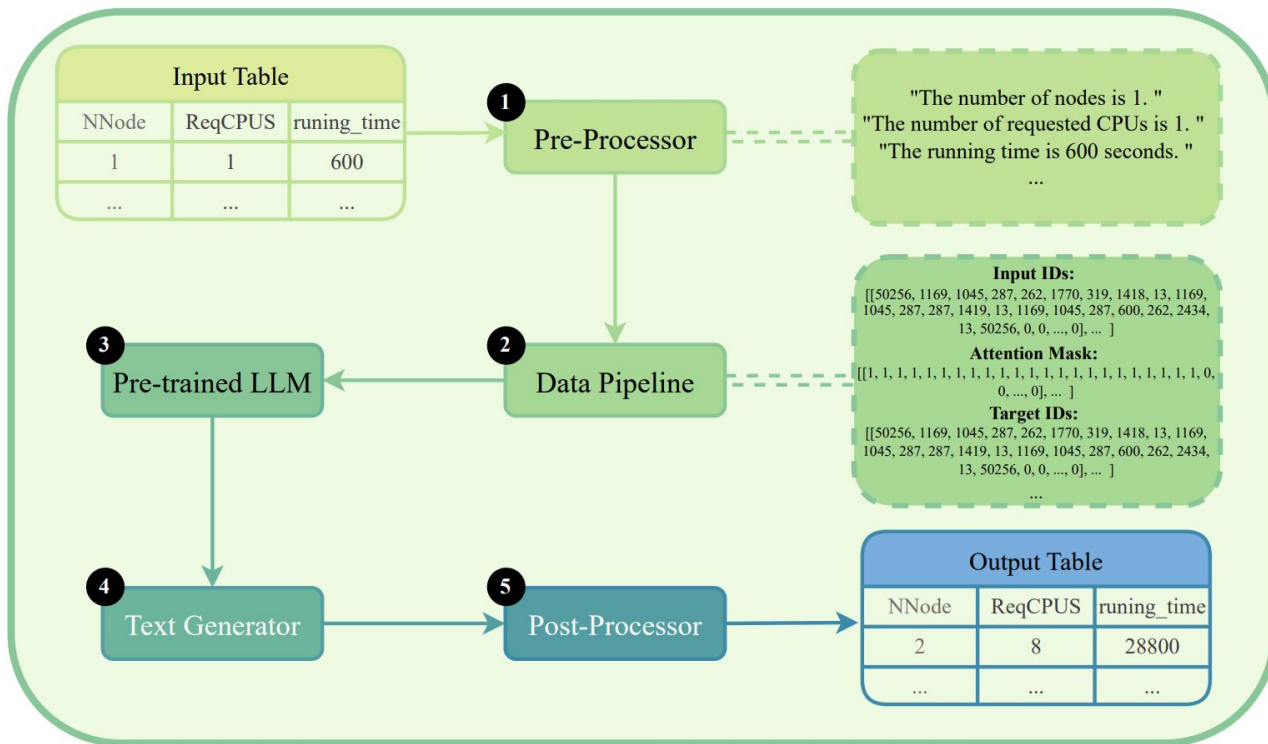
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RQ2.1



Design - How to Use LLMs for Job Data Synthesis?

RQ2.1



- **Baseline Models:** TabGAN & CTGAN

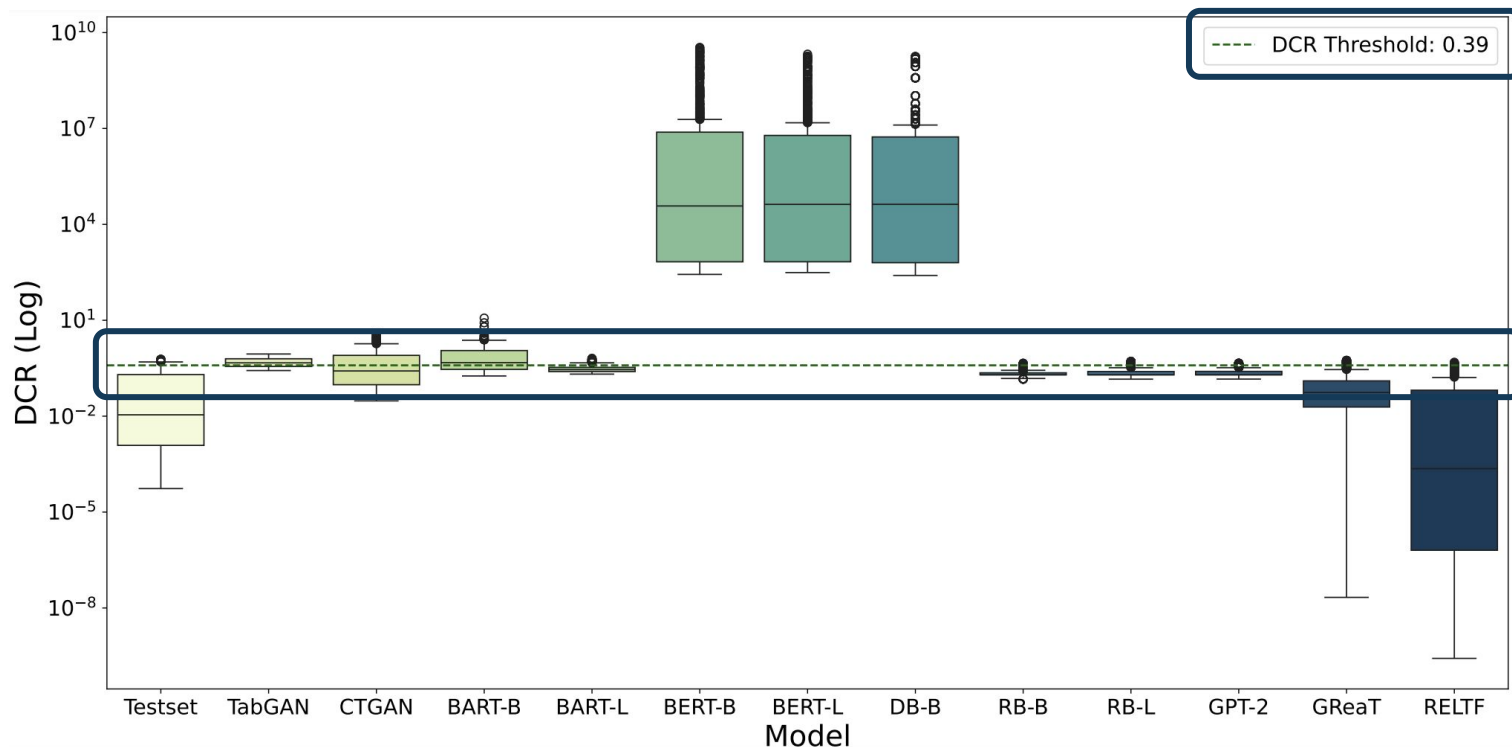
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 - Measures the **similarity**

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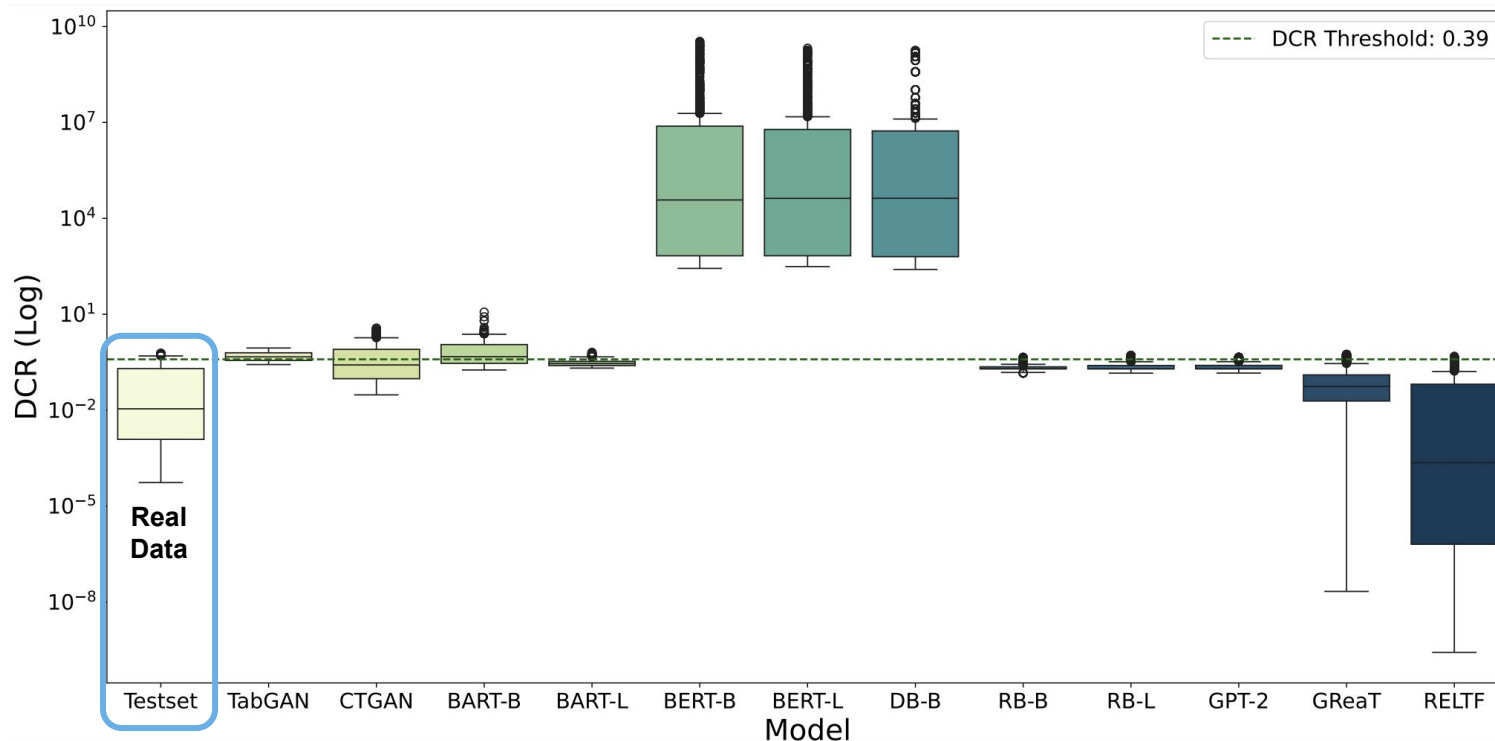
Evaluation (2/3) - Distance to the Closest Record

RQ2.2



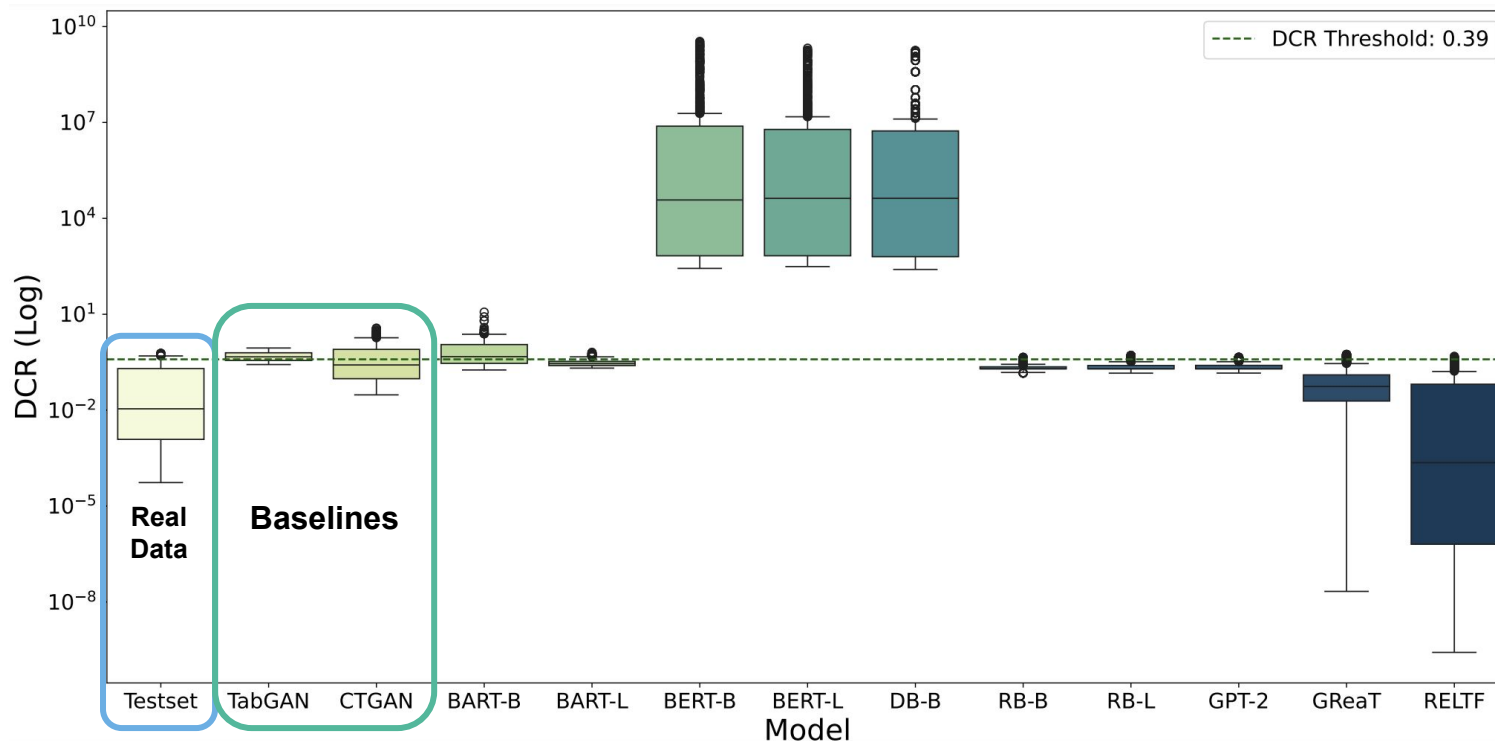
Evaluation (2/3) - Distance to the Closest Record

RQ2.2



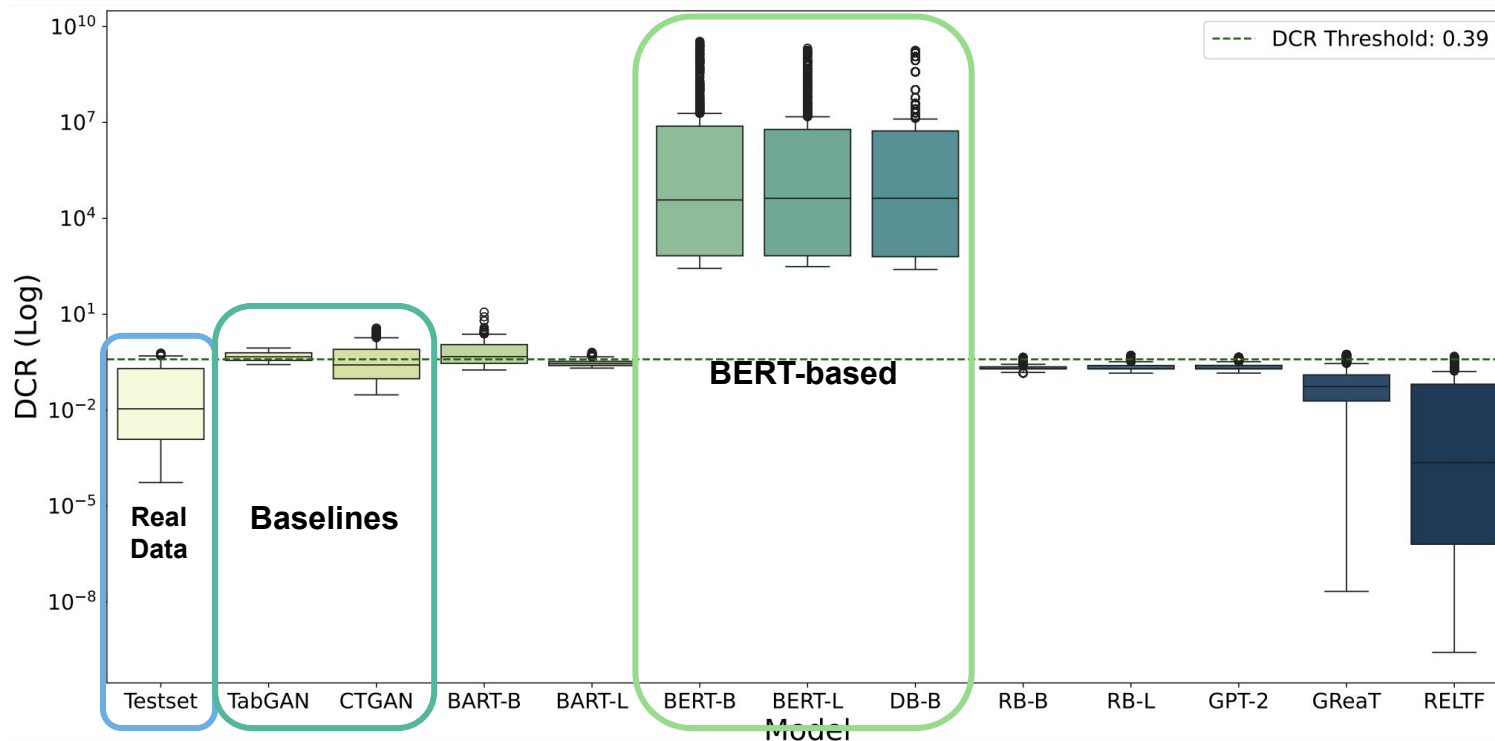
Evaluation (2/3) - Distance to the Closest Record

RQ2.2



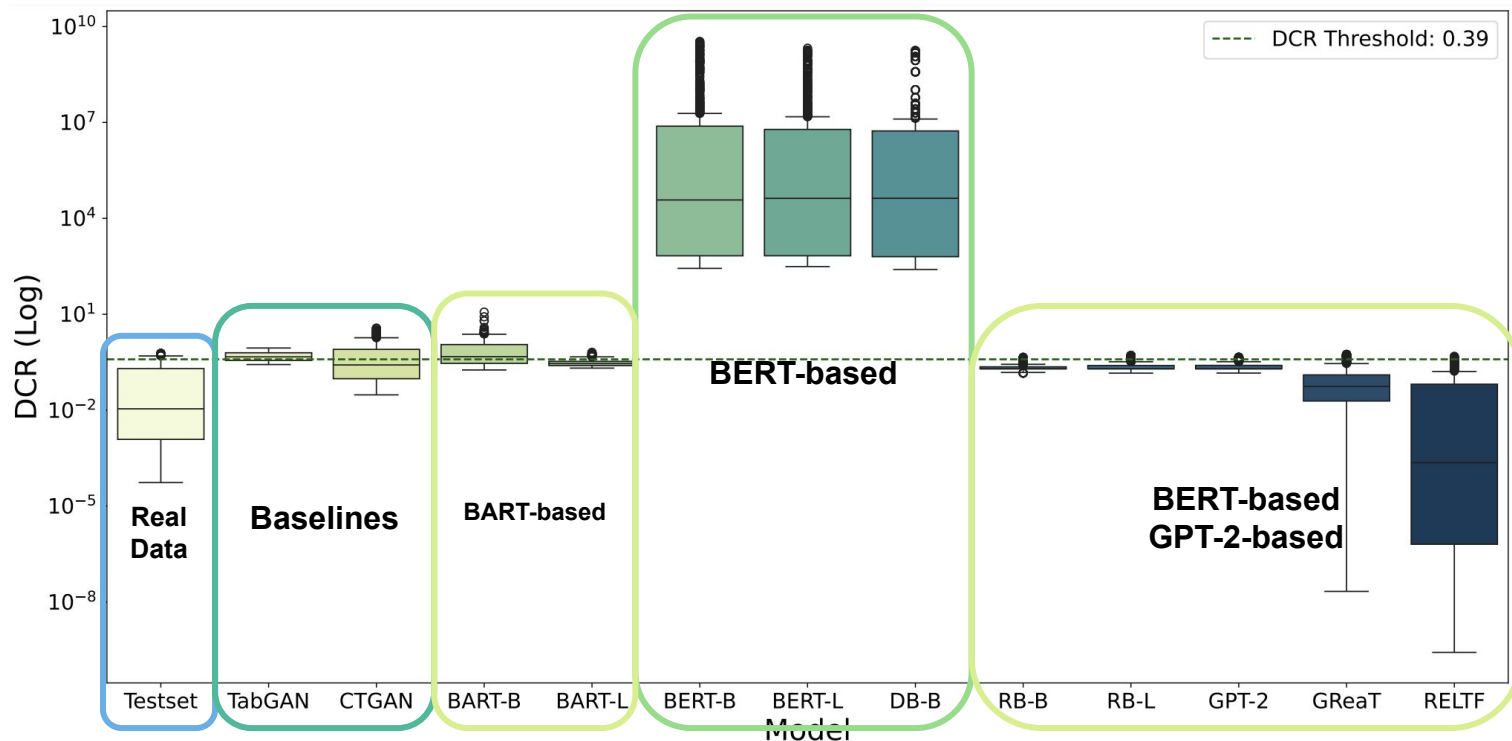
Evaluation (2/3) - Distance to the Closest Record

RQ2.2



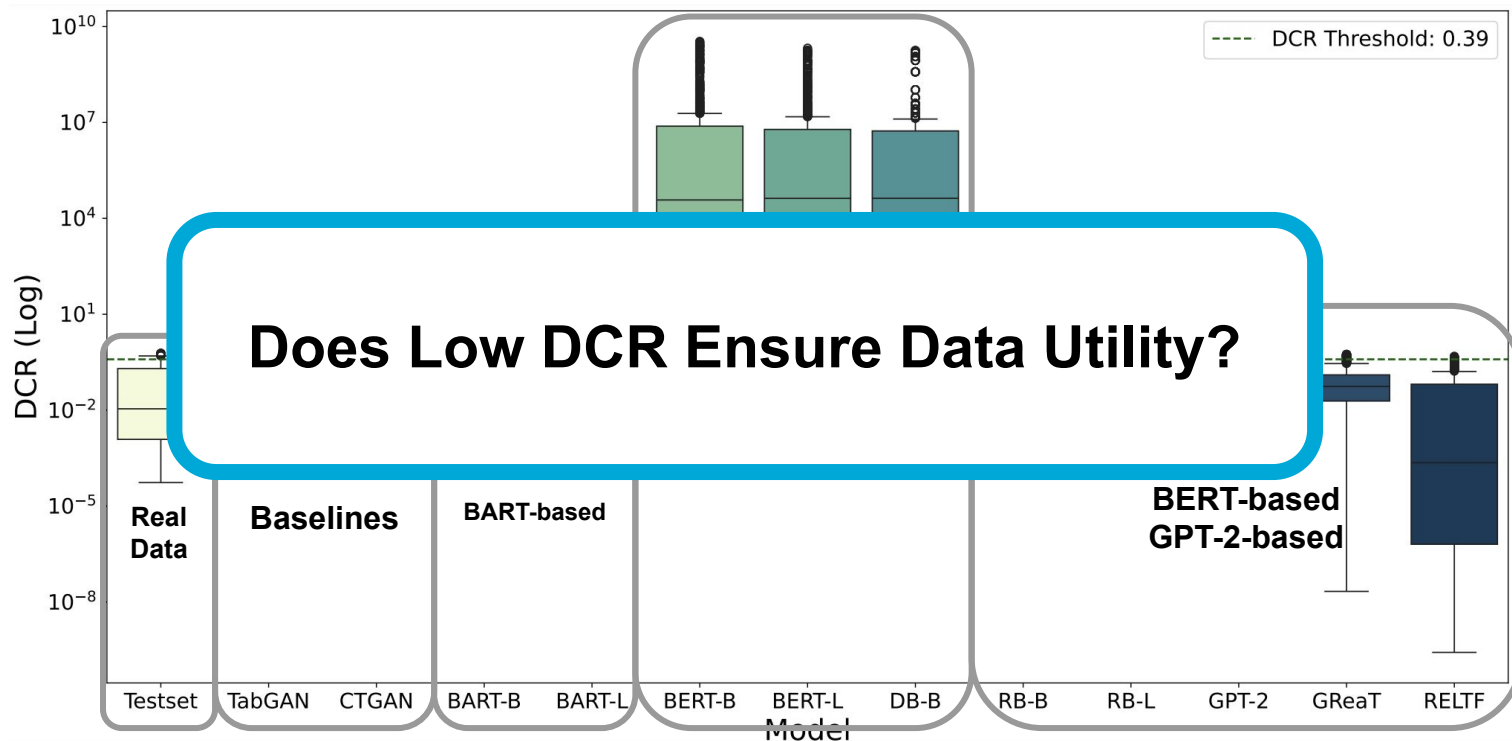
Evaluation (2/3) - Distance to the Closest Record

RQ2.2



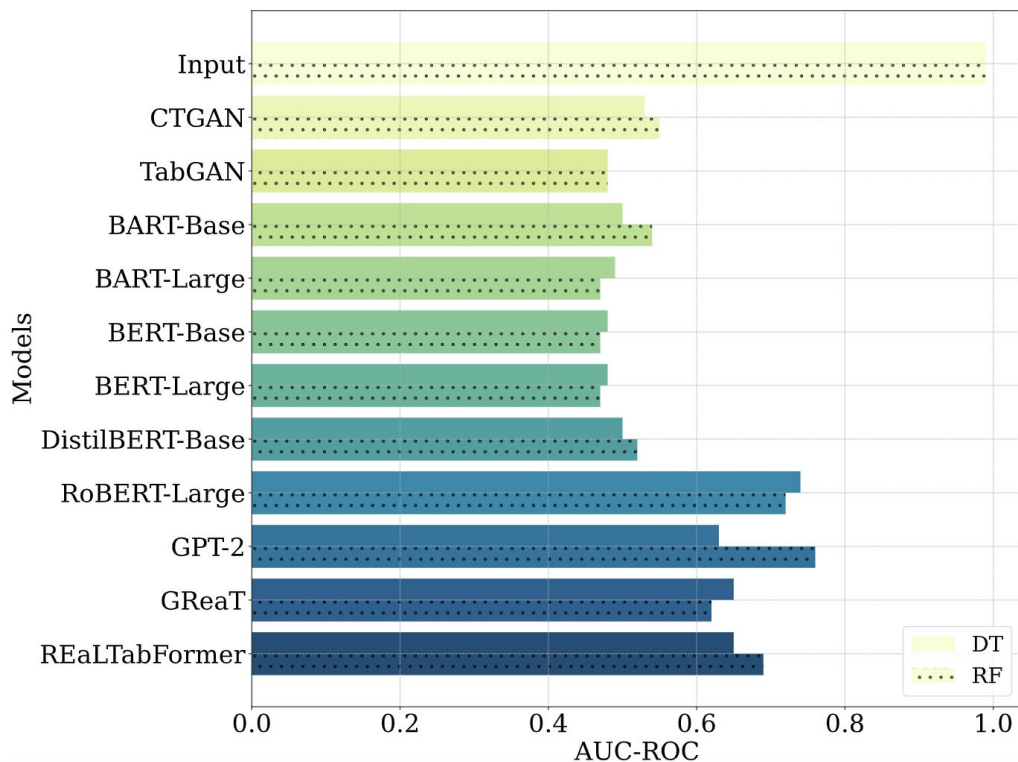
Evaluation (2/3) - Distance to the Closest Record

RQ2.2



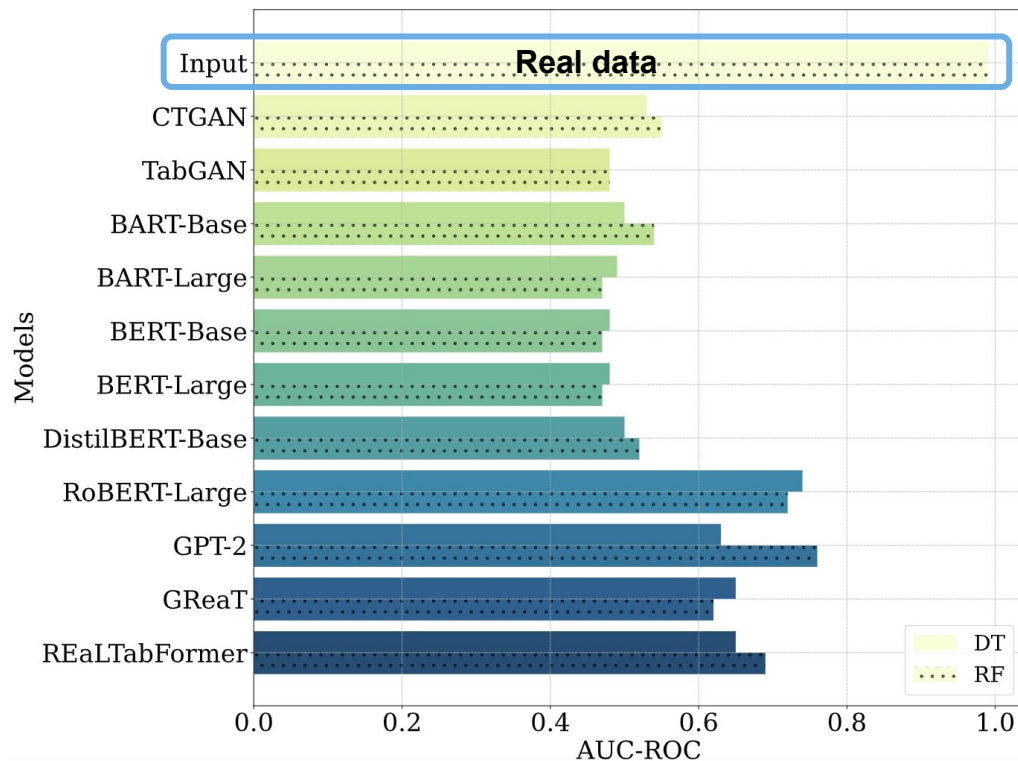
Evaluation (3/3) - Machine Learning Efficiency

RQ2.2



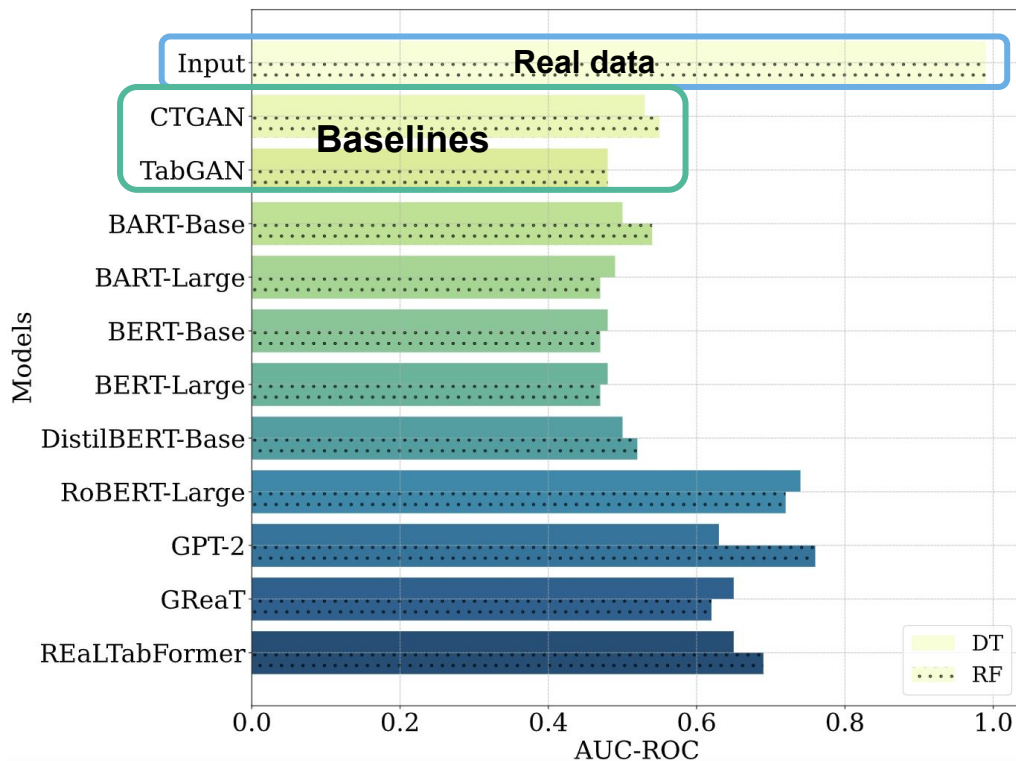
Evaluation (3/3) - Machine Learning Efficiency

RQ2.2



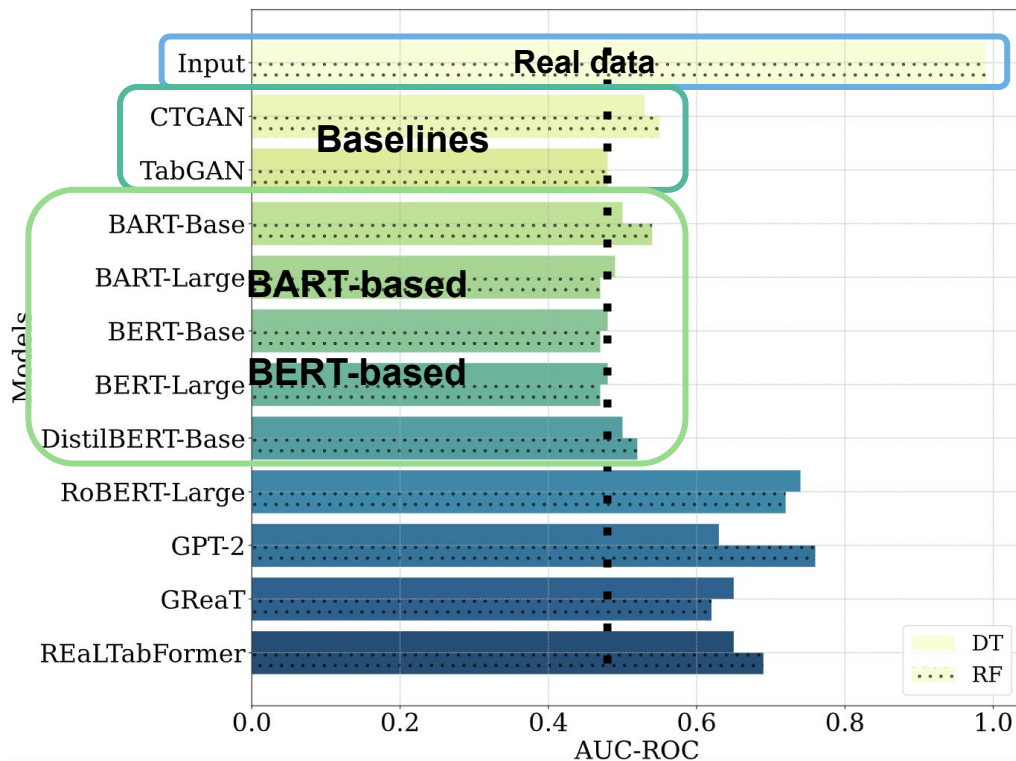
Evaluation (3/3) - Machine Learning Efficiency

RQ2.2



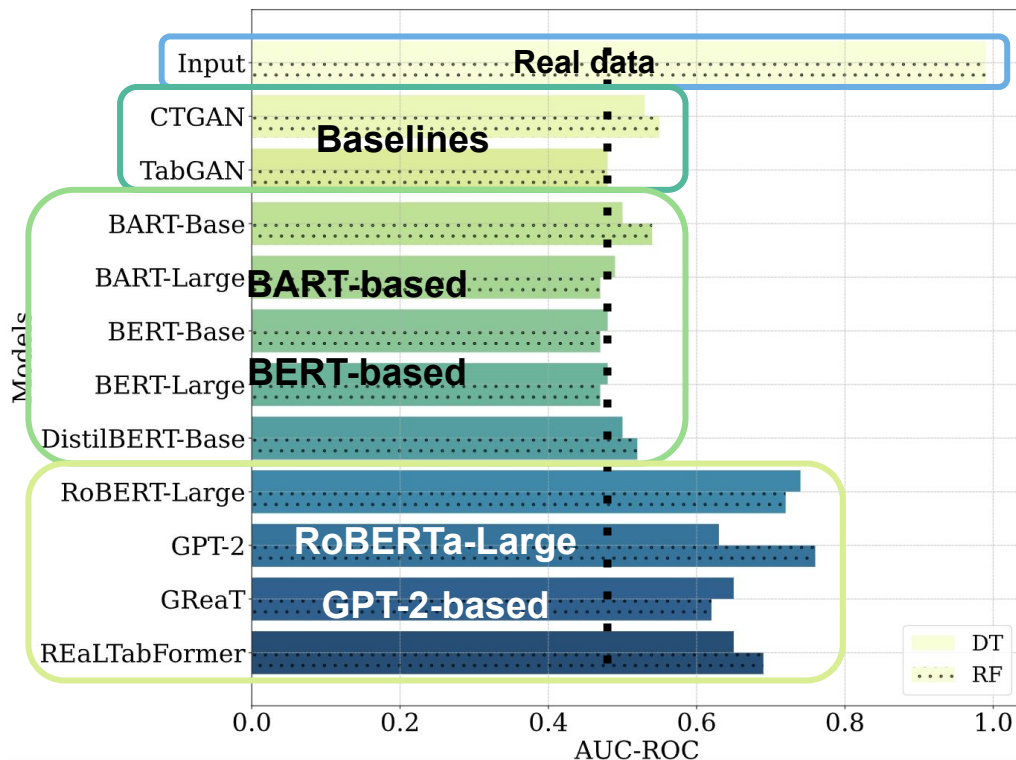
Evaluation (3/3) - Machine Learning Efficiency

RQ2.2



Evaluation (3/3) - Machine Learning Efficiency

RQ2.2



- **F1** (DCR) - **RoBERTa-Large** and **GPT-2-based models** demonstrate the most promise with low DCR values.
- **F2** (MLE) - Predictive models trained on synthetic datasets show **varied performance**, falling short compared to real data.
- **F3** - There is a need for **improvements** in synthetic data generation techniques.

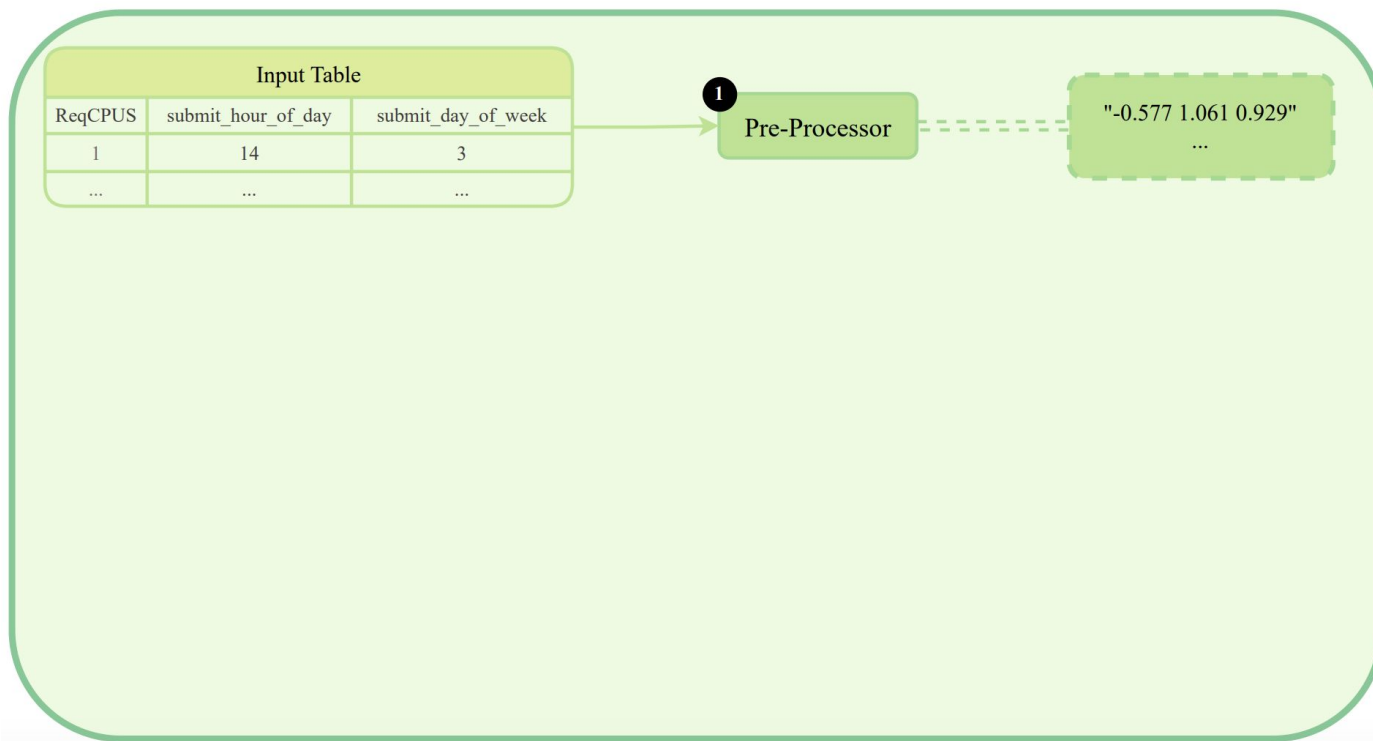
Design - How to Use LLMs to Predict Job End-State?

RQ3.1

Input Table		
ReqCPUS	submit_hour_of_day	submit_day_of_week
1	14	3
...

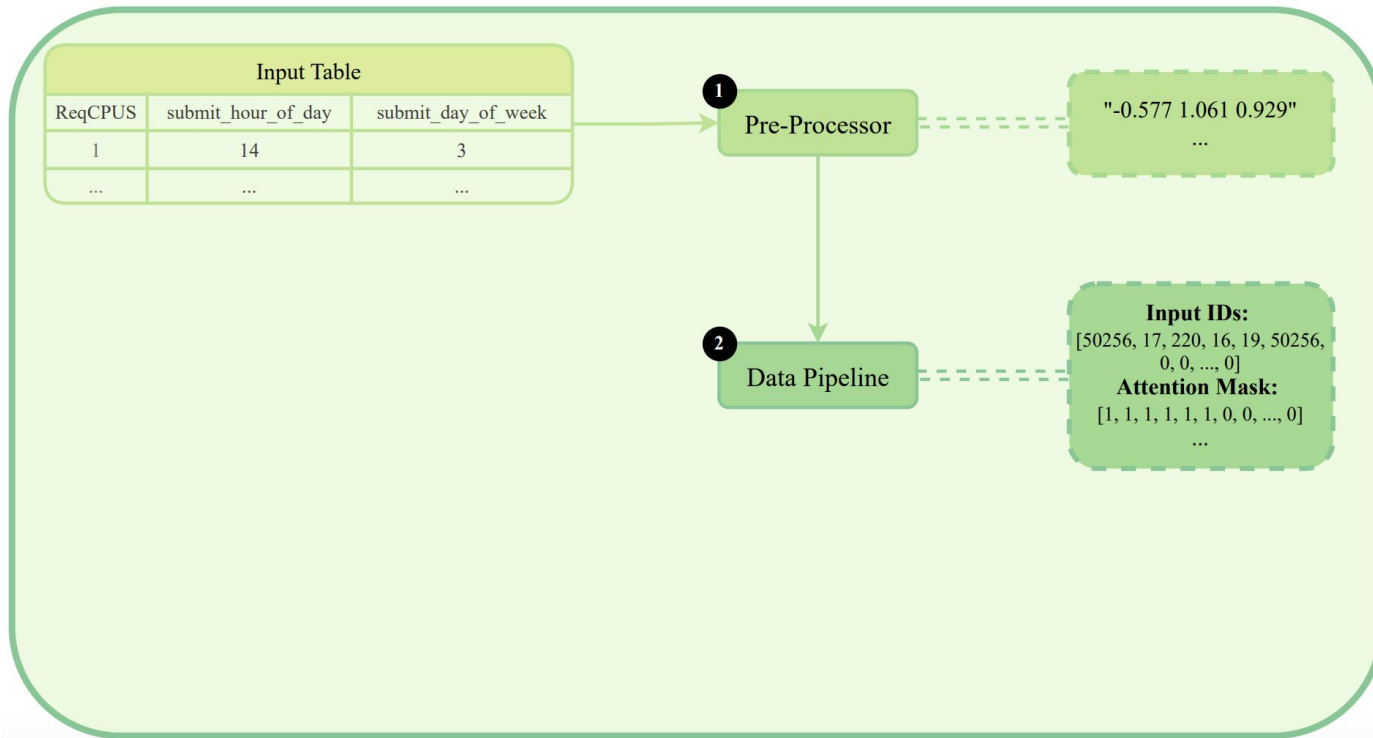
Design - How to Use LLMs to Predict Job End-State?

RQ3.1



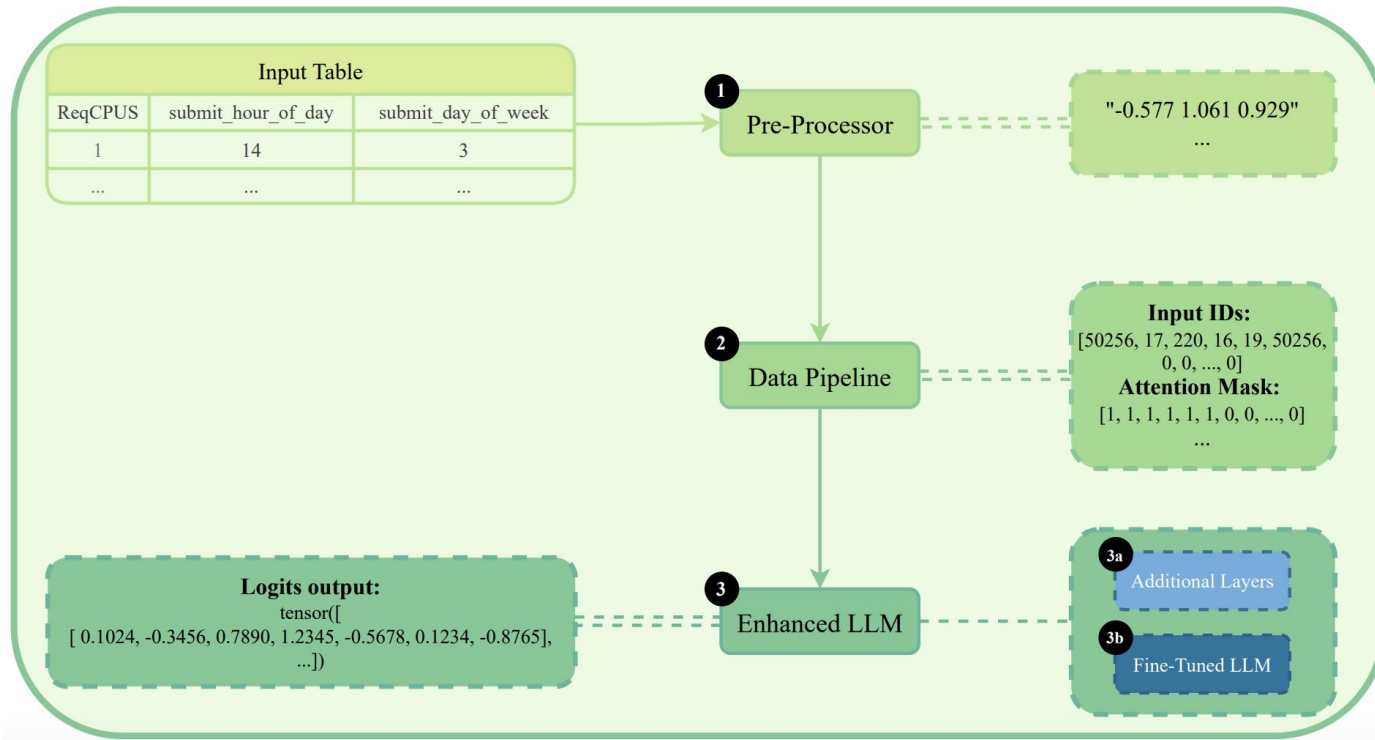
Design - How to Use LLMs to Predict Job End-State?

RQ3.1



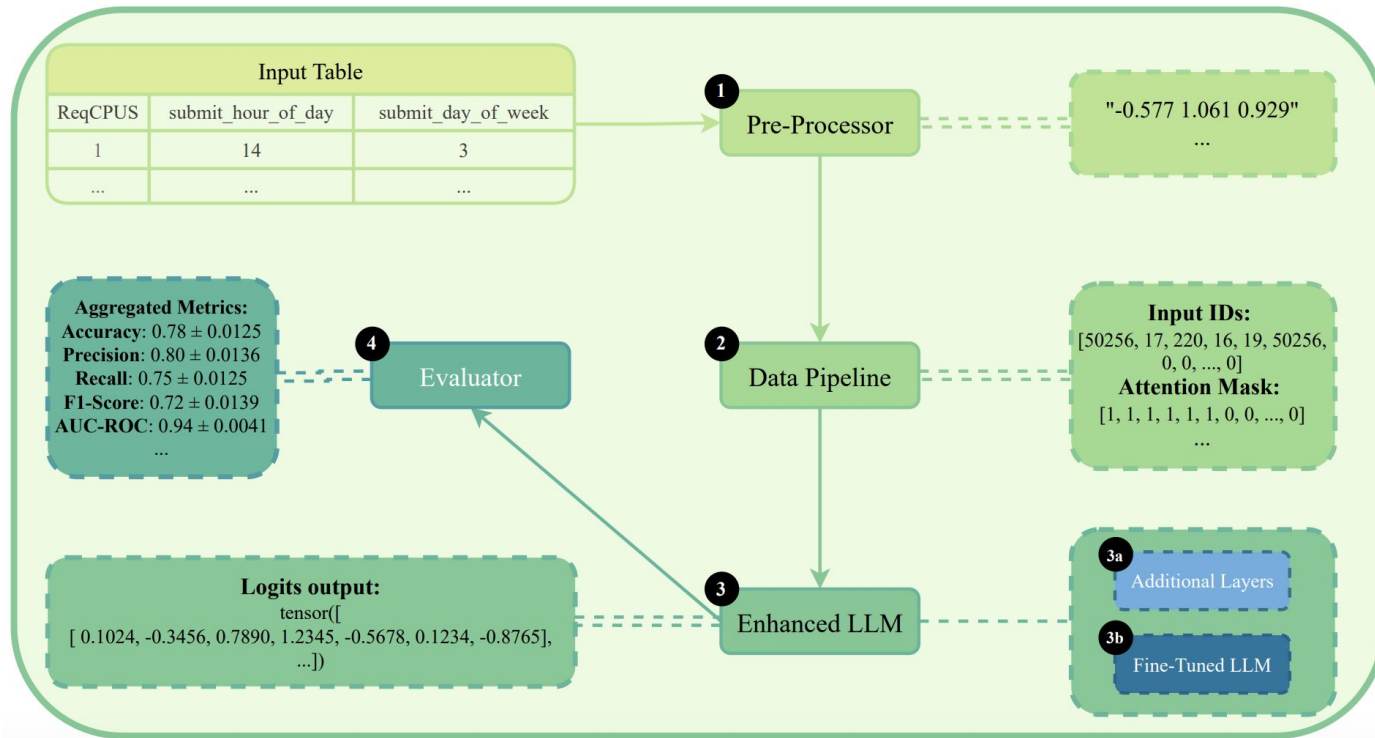
Design - How to Use LLMs to Predict Job End-State?

RQ3.1



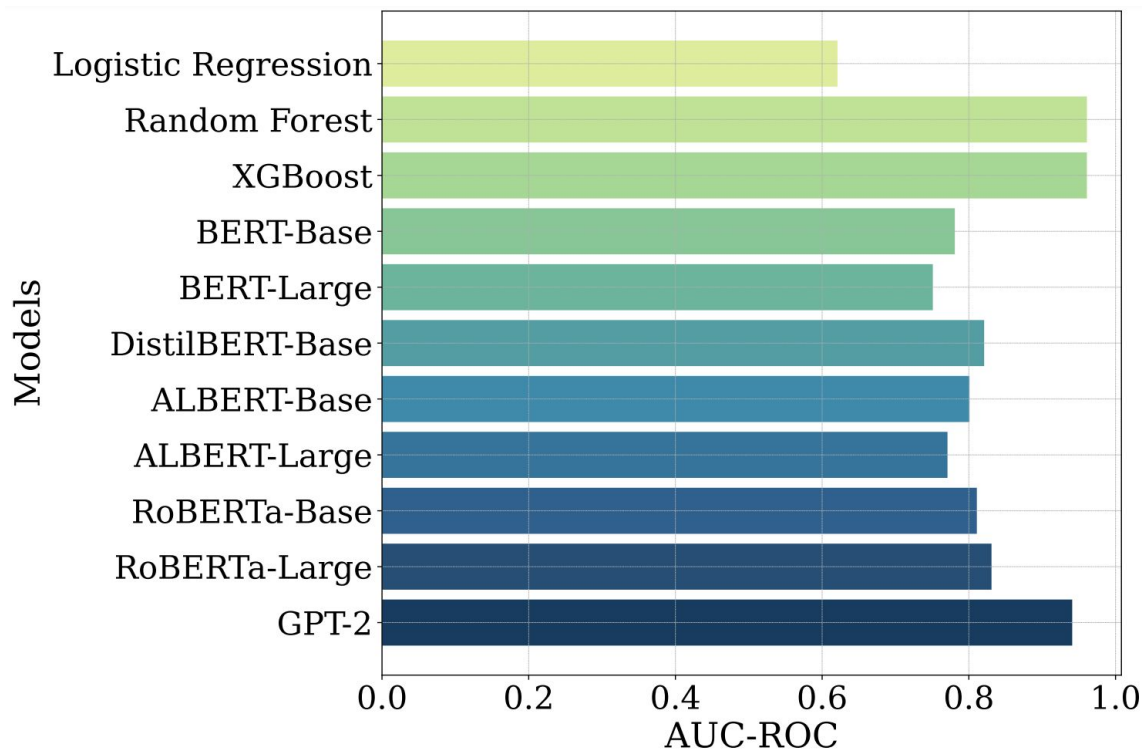
Design - How to Use LLMs to Predict Job End-State?

RQ3.1



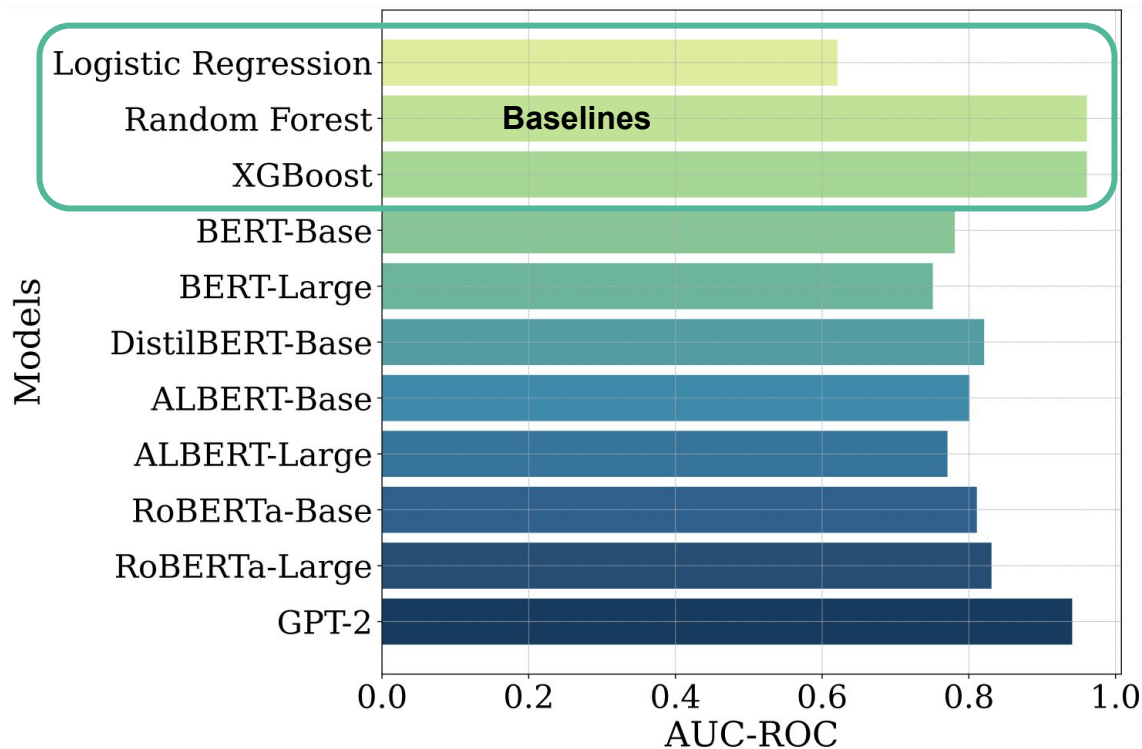
Evaluation - How Well Do LLMs Work in Prediction?

RQ3.2



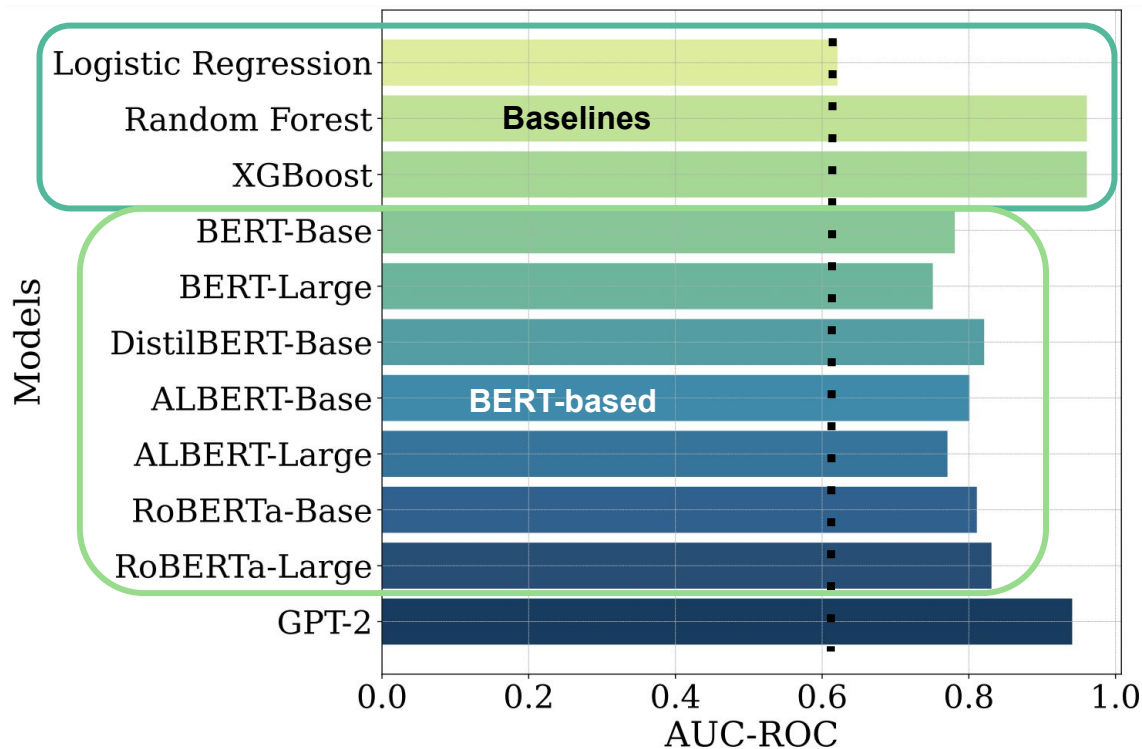
Evaluation - How Well Do LLMs Work in Prediction?

RQ3.2



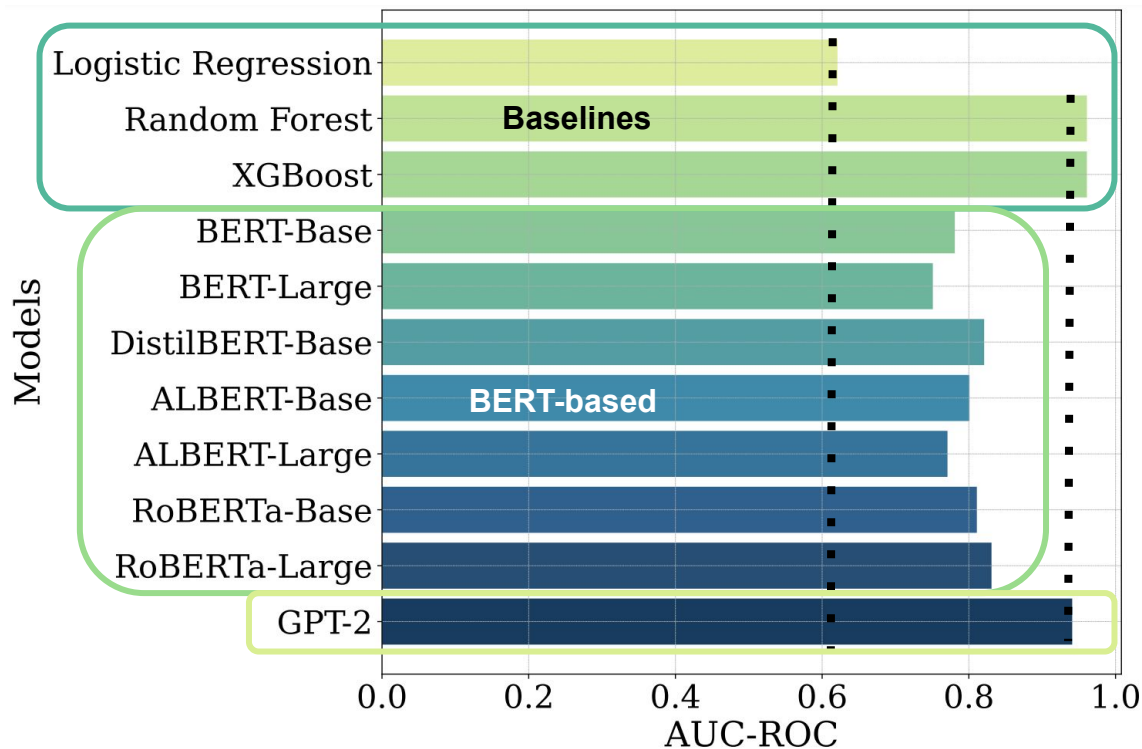
Evaluation - How Well Do LLMs Work in Prediction?

RQ3.2



Evaluation - How Well Do LLMs Work in Prediction?

RQ3.2



- **F1 - GPT-2** shows competitive performance against the best-performing traditional models.
- **F2 - RoBERTa-Large** and **DistilBERT-Base** also show promising results.
- **F3 - LLMs** demonstrate **significant potential** in predicting job termination states within HPC clusters.

Conclusion & Future Work

- Existing LLM applications primarily focus on **programming-related tasks**.
- Significant **potential** in workload synthesis and predictive analysis.

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- Other LLMs show varying levels of effectiveness.

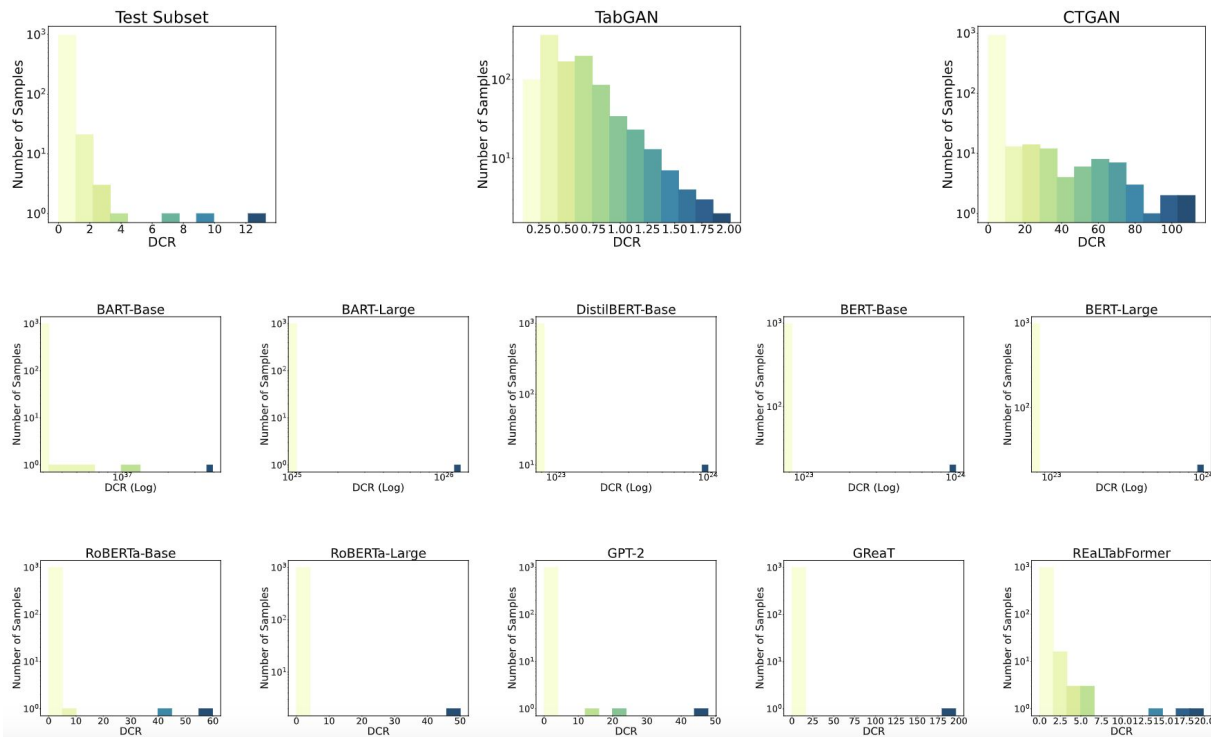
Conclusion & Future Work

- Existing LLM applications primarily focus on **programming-related tasks**.
- Significant **potential** in workload synthesis and predictive analysis.
- Models such as GPT-2 show promising results in predictive tasks.
- LLM-generated synthetic data for training predictive models.
- **Future Work**
 - A wider range of LLM architectures.
 - Additional metrics for synthetic data evaluation.
 - Advanced techniques for textual encoding.
- **GPT-2** shows promising results in predictive tasks.
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Backup Slides

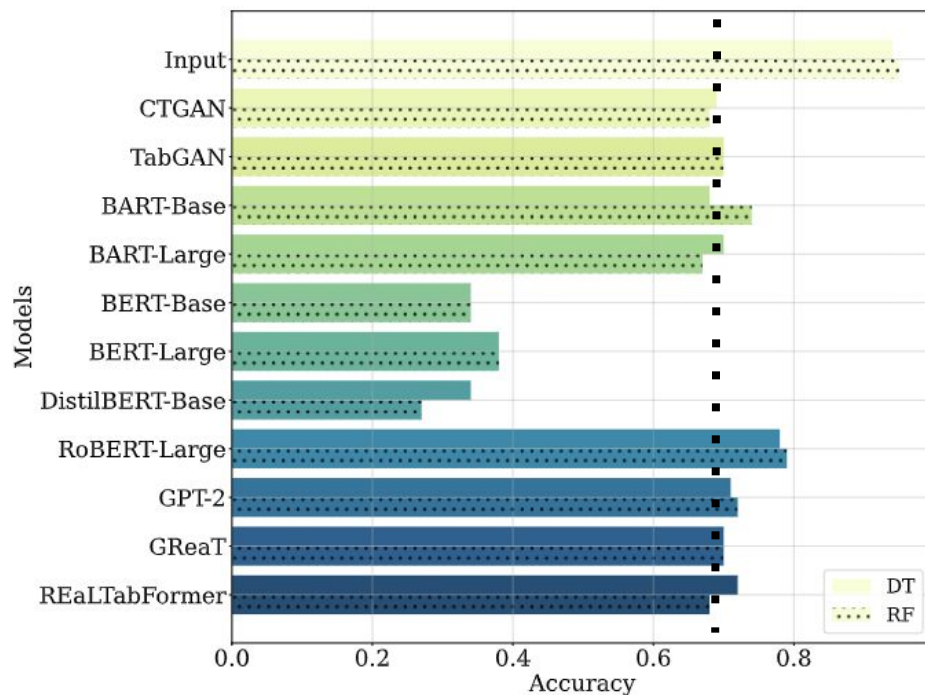
DCR Distributions

RQ2.2



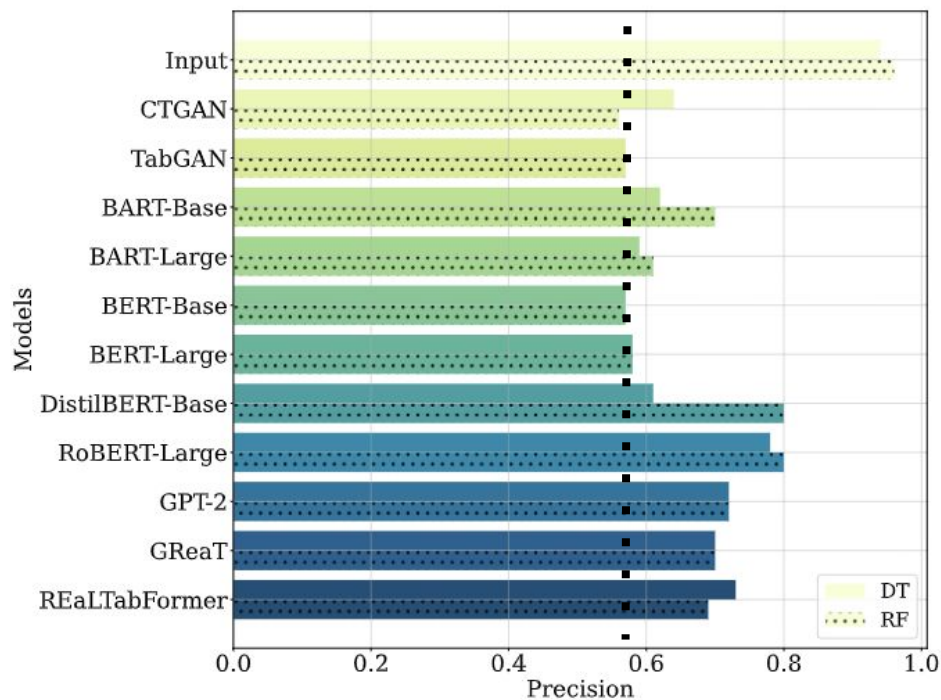
MLE Metrics (1/4) - Accuracy

RQ2.2



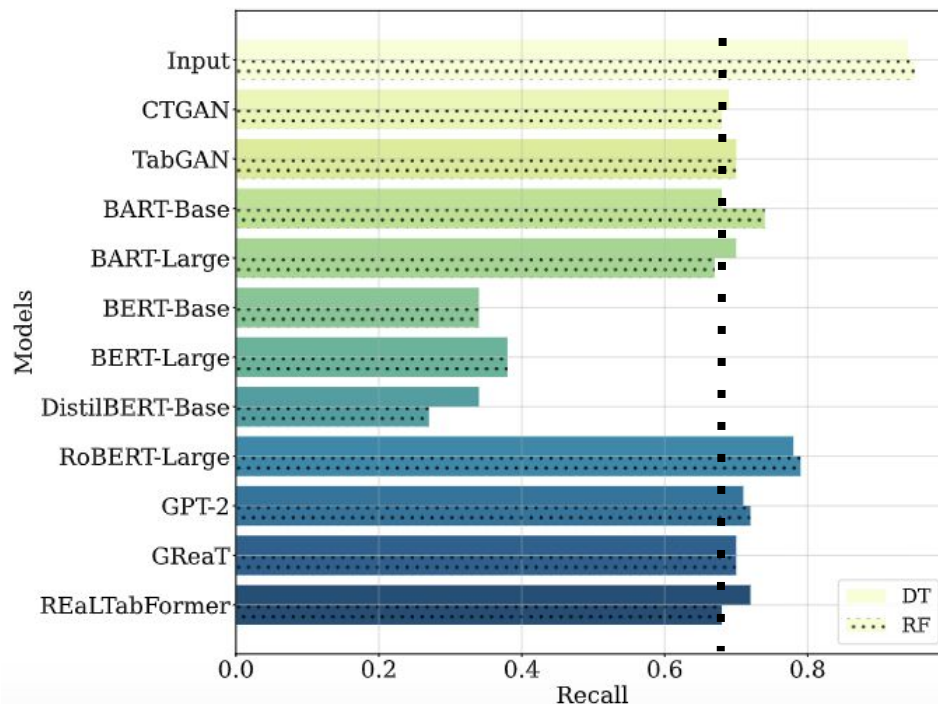
MLE Metrics (2/4) - Precision

RQ2.2



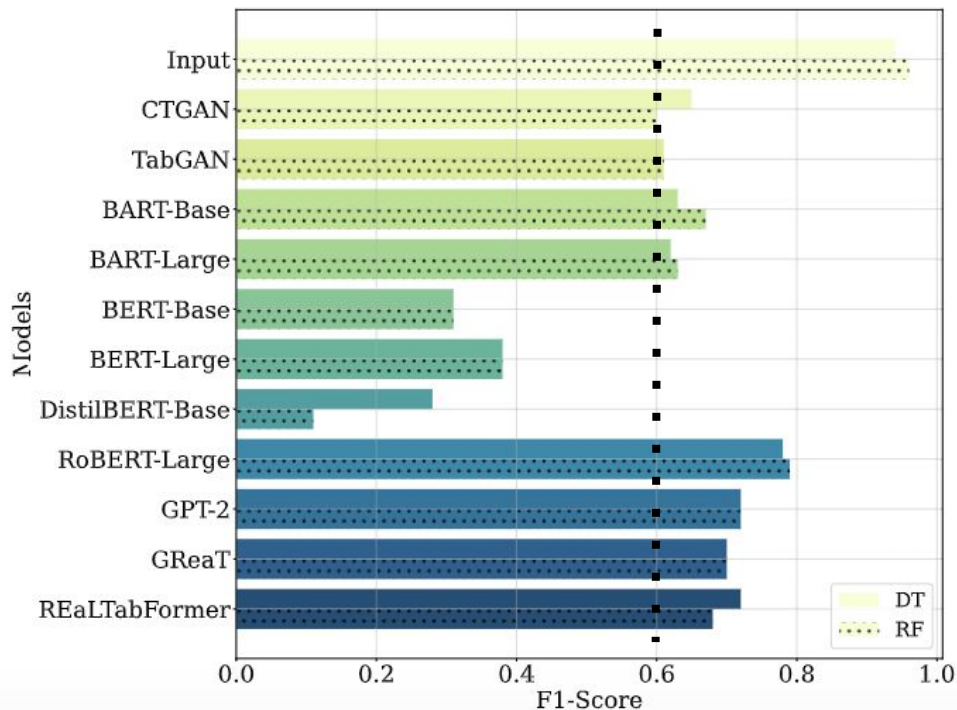
MLE Metrics (3/4) - Recall

RQ2.2



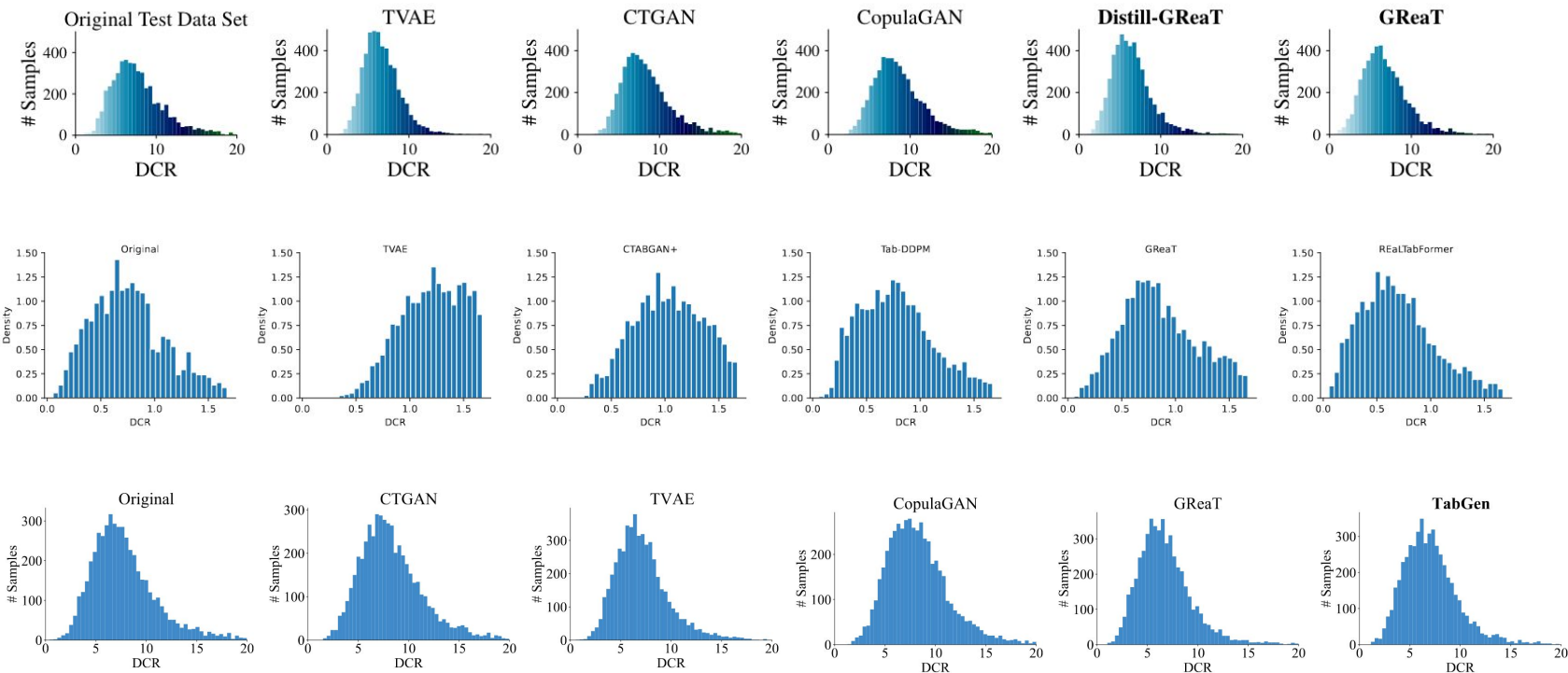
MLE Metrics (4/4) - F1 - Score

RQ2.2



DCR Distribution

RQ2.2



LLMs in Classification

RQ3.2

Dataset	Method	Number of Shots									
		0	4	8	16	32	64	128	256	512	all
Bank	XGBoost	—	0.50 ₀₀	0.56 ₀₉	0.68 ₀₄	0.76 ₀₃	0.83 ₀₂	0.85 ₀₃	0.88 ₀₁	0.90 ₀₁	0.94 ₀₀
	TabPFN	—	0.59 ₁₄	0.66 ₀₈	0.69 ₀₂	0.76 ₀₃	0.82 ₀₃	0.86 ₀₂	0.89 ₀₀	0.90 ₀₀	0.91 ₀₀
	TabLLM	0.63 ₀₁	0.59 ₁₀	0.64 ₀₅	0.65 ₀₅	0.64 ₀₆	0.69 ₀₃	0.82 ₀₅	0.87 ₀₁	0.88 ₀₁	0.92 _†
Blood	XGBoost	—	0.50 ₀₀	0.58 ₀₇	0.66 ₀₄	0.67 ₀₆	0.68 ₀₅	0.71 ₀₆	0.70 ₀₇	0.67 ₀₆	0.71 ₀₄
	TabPFN	—	0.52 ₀₈	0.64 ₀₄	0.67 ₀₁	0.70 ₀₄	0.73 ₀₄	0.75 ₀₄	0.76 ₀₄	0.76 ₀₃	0.74 ₀₃
	TabLLM	0.61 ₀₄	0.58 ₀₉	0.66 ₀₃	0.66 ₀₇	0.68 ₀₄	0.68 ₀₄	0.68 ₀₆	0.70 ₀₈	0.68 ₀₄	0.70 ₀₄
Calhousing	XGBoost	—	0.50 ₀₀	0.62 ₁₀	0.74 ₀₃	0.79 ₀₄	0.82 ₀₄	0.87 ₀₁	0.90 ₀₁	0.92 ₀₁	0.97 ₀₀
	TabPFN	—	0.63 ₁₃	0.63 ₁₁	0.80 ₀₃	0.85 ₀₃	0.89 ₀₁	0.91 ₀₁	0.92 ₀₀	0.93 ₀₀	0.94 ₀₀
	TabLLM	0.61 ₀₁	0.63 ₀₅	0.60 ₀₇	0.70 ₀₈	0.77 ₀₈	0.77 ₀₄	0.81 ₀₂	0.83 ₀₁	0.86 ₀₂	0.95 ₀₀
Car	XGBoost	—	0.50 ₀₀	0.59 ₀₄	0.70 ₀₈	0.82 ₀₃	0.91 ₀₂	0.95 ₀₁	0.98 ₀₁	0.99 ₀₁	1.00 ₀₀
	TabPFN	—	0.64 ₀₆	0.75 ₀₅	0.87 ₀₄	0.92 ₀₂	0.97 ₀₀	0.99 ₀₁	1.00 ₀₀	1.00 ₀₀	1.00 ₀₀
	TabLLM	0.82 ₀₂	0.83 ₀₃	0.85 ₀₃	0.86 ₀₃	0.91 ₀₂	0.96 ₀₂	0.98 ₀₁	0.99 ₀₀	1.00 ₀₀	1.00 ₀₀
Credit-g	XGBoost	—	0.50 ₀₀	0.51 ₀₇	0.59 ₀₅	0.66 ₀₃	0.67 ₀₆	0.68 ₀₂	0.73 ₀₂	0.75 ₀₃	0.78 ₀₄
	TabPFN	—	0.58 ₀₈	0.59 ₀₃	0.64 ₀₆	0.69 ₀₇	0.70 ₀₇	0.72 ₀₆	0.75 ₀₄	0.75 ₀₂	0.75 ₀₃
	TabLLM	0.53 ₀₅	0.69 ₀₄	0.66 ₀₄	0.66 ₀₅	0.72 ₀₆	0.70 ₀₇	0.71 ₀₇	0.72 ₀₃	0.72 ₀₂	0.70 ₀₂
Diabetes	XGBoost	—	0.50 ₀₀	0.59 ₁₆	0.72 ₀₇	0.69 ₀₈	0.73 ₀₅	0.78 ₀₅	0.80 ₀₃	0.80 ₀₁	0.84 ₀₃
	TabPFN	—	0.61 ₁₃	0.67 ₁₁	0.71 ₀₇	0.77 ₀₃	0.82 ₀₃	0.83 ₀₃	0.83 ₀₃	0.81 ₀₂	0.81 ₀₃
	TabLLM	0.68 ₀₆	0.61 ₀₉	0.63 ₀₈	0.69 ₀₇	0.68 ₀₄	0.73 ₀₃	0.79 ₀₄	0.78 ₀₂	0.78 ₀₄	0.80 ₀₄
Heart	XGBoost	—	0.50 ₀₀	0.55 ₁₄	0.84 ₀₇	0.88 ₀₄	0.91 ₀₁	0.91 ₀₁	0.90 ₀₁	0.92 ₀₁	0.94 ₀₁
	TabPFN	—	0.84 ₀₆	0.88 ₀₅	0.87 ₀₆	0.91 ₀₂	0.92 ₀₂	0.92 ₀₂	0.92 ₀₁	0.92 ₀₂	0.92 ₀₂
	TabLLM	0.54 ₀₄	0.76 ₁₄	0.83 ₀₅	0.87 ₀₄	0.87 ₀₆	0.91 ₀₁	0.90 ₀₁	0.92 ₀₁	0.92 ₀₁	0.94 ₀₁
Income	XGBoost	—	0.50 ₀₀	0.59 ₀₆	0.77 ₀₂	0.79 ₀₃	0.82 ₀₂	0.84 ₀₁	0.87 ₀₁	0.88 ₀₀	0.93 ₀₀
	TabPFN	—	0.73 ₀₀	0.71 ₀₇	0.75 ₀₇	0.80 ₀₁	0.82 ₀₁	0.84 ₀₀	0.86 ₀₁	0.87 ₀₁	0.89 ₀₀
	TabLLM	0.84 ₀₀	0.84 ₀₁	0.84 ₀₂	0.84 ₀₄	0.84 ₀₁	0.84 ₀₂	0.86 ₀₁	0.87 ₀₀	0.89 ₀₁	0.92 ₀₀
Jungle	XGBoost	—	0.50 ₀₀	0.58 ₀₇	0.72 ₀₅	0.78 ₀₃	0.81 ₀₂	0.84 ₀₂	0.87 ₀₁	0.91 ₀₁	0.98 ₀₀
	TabPFN	—	0.65 ₀₈	0.72 ₀₄	0.71 ₀₇	0.78 ₀₂	0.81 ₀₁	0.84 ₀₁	0.88 ₀₁	0.91 ₀₀	0.93 ₀₀
	TabLLM	0.60 ₀₀	0.64 ₀₁	0.64 ₀₂	0.65 ₀₃	0.71 ₀₂	0.78 ₀₂	0.81 ₀₂	0.84 ₀₁	0.89 ₀₁	1.00 _†

#Shots	Method	Bank	Blood	C. Hous.	Car	Creditg	Diabetes	Heart	Income	Jungle
64	Logistic Reg.	0.84 ₀₂	0.74 ₀₂	0.88 ₀₁	0.93 ₀₂	0.66 ₀₇	0.80 ₀₂	0.91 ₀₁	0.83 ₀₃	0.79 ₀₁
	LightGBM	0.77 ₀₃	0.69 ₀₄	0.81 ₀₂	0.85 ₀₆	0.61 ₀₉	0.79 ₀₂	0.91 ₀₁	0.78 ₀₃	0.79 ₀₂
	XGBoost	0.83 ₀₂	0.68 ₀₅	0.82 ₀₄	0.91 ₀₂	0.67 ₀₆	0.73 ₀₅	0.91 ₀₁	0.82 ₀₂	0.81 ₀₂
	SAINT	0.81 ₀₃	0.67 ₀₅	0.81 ₀₂	0.92 ₀₂	0.66 ₀₆	0.79 ₀₃	0.90 ₀₄	0.84 ₀₂	0.81 ₀₁
	TabNet	0.71 ₀₆	0.63 ₀₆	0.72 ₀₃	0.73 ₀₇	0.56 ₀₅	0.71 ₀₄	0.83 ₀₅	0.71 ₀₄	0.73 ₀₄
	NODE	0.78 ₀₂	0.71 ₀₅	0.80 ₀₁	0.80 ₀₂	0.63 ₀₄	0.77 ₀₄	0.88 ₀₂	0.75 ₀₂	0.75 ₀₄
	TabPFN	0.82 ₀₃	0.73 ₀₄	0.89 ₀₁	0.97 ₀₀	0.70 ₀₇	0.82 ₀₃	0.92 ₀₂	0.82 ₀₄	0.81 ₀₁
	TabLLM	0.69 ₀₃	0.68 ₀₄	0.77 ₀₄	0.96 ₀₂	0.70 ₀₇	0.73 ₀₃	0.91 ₀₁	0.84 ₀₂	0.78 ₀₂
	LLaMA	0.62 ₀₂	0.66 ₀₃	0.57 ₀₄	0.90 ₀₂	0.67 ₀₉	0.78 ₀₅	0.88 ₀₂	0.78 ₀₅	0.63 ₀₄
	LLaMA-GTL	0.86 ₀₁	0.72 ₀₅	0.78 ₀₄	0.96 ₀₁	0.70 ₀₉	0.83 ₀₄	0.88 ₀₅	0.84 ₀₁	0.69 ₀₄
	Logistic Reg.	0.89 ₀₀	0.76 ₀₃	0.91 ₀₀	0.98 ₀₀	0.76 ₀₂	0.83 ₀₂	0.93 ₀₁	0.88 ₀₀	0.80 ₀₀
	LightGBM	0.89 ₀₀	0.67 ₀₅	0.92 ₀₀	0.99 ₀₁	0.75 ₀₂	0.79 ₀₃	0.92 ₀₁	0.88 ₀₀	0.91 ₀₀
512	XGBoost	0.90 ₀₁	0.67 ₀₆	0.92 ₀₁	0.99 ₀₁	0.75 ₀₃	0.80 ₀₁	0.92 ₀₁	0.88 ₀₀	0.91 ₀₁
	SAINT	0.88 ₀₁	0.73 ₀₂	0.91 ₀₂	0.99 ₀₀	0.73 ₀₃	0.77 ₀₃	0.92 ₀₁	0.88 ₀₀	0.90 ₀₀
	TabNet	0.83 ₀₃	0.72 ₀₂	0.87 ₀₁	0.98 ₀₁	0.66 ₀₄	0.74 ₀₇	0.88 ₀₃	0.83 ₀₂	0.84 ₀₁
	NODE	0.86 ₀₁	0.76 ₀₃	0.87 ₀₁	0.96 ₀₁	0.70 ₀₂	0.83 ₀₂	0.92 ₀₃	0.83 ₀₁	0.80 ₀₀
	TabPFN	0.90 ₀₀	0.76 ₀₃	0.93 ₀₀	1.00 ₀₀	0.75 ₀₂	0.81 ₀₂	0.92 ₀₂	0.87 ₀₁	0.91 ₀₀
	TabLLM	0.88 ₀₁	0.68 ₀₄	0.86 ₀₂	1.00 ₀₀	0.72 ₀₂	0.78 ₀₄	0.92 ₀₁	0.89 ₀₁	0.89 ₀₁
	LLaMA	0.77 ₀₂	0.72 ₀₅	0.86 ₀₂	0.99 ₀₀	0.72 ₀₄	0.83 ₀₄	0.92 ₀₂	0.89 ₀₁	0.85 ₀₃
	LLaMA-GTL	0.90 ₀₀	0.75 ₀₄	0.89 ₀₂	0.99 ₀₁	0.74 ₀₅	0.85 ₀₃	0.93 ₀₂	0.89 ₀₁	0.89 ₀₁
	Logistic Reg.	0.91 ₀₀	0.76 ₀₃	0.92 ₀₀	0.98 ₀₀	0.79 ₀₃	0.83 ₀₂	0.93 ₀₁	0.90 ₀₀	0.81 ₀₀
	LightGBM	0.94 ₀₀	0.74 ₀₄	0.97 ₀₀	1.00 ₀₀	0.78 ₀₂	0.83 ₀₃	0.94 ₀₁	0.93 ₀₀	0.98 ₀₀
	XGBoost	0.94 ₀₀	0.71 ₀₄	0.97 ₀₀	1.00 ₀₀	0.78 ₀₄	0.84 ₀₃	0.94 ₀₁	0.93 ₀₀	0.98 ₀₀
	SAINT	0.93 ₀₀	0.74 ₀₃	0.95 ₀₀	1.00 ₀₀	0.77 ₀₄	0.83 ₀₃	0.93 ₀₁	0.91 ₀₀	1.00 ₀₀
All	TabNet	0.93 ₀₀	0.71 ₀₃	0.96 ₀₀	1.00 ₀₀	0.64 ₀₃	0.81 ₀₃	0.89 ₀₃	0.92 ₀₀	0.99 ₀₀
	NODE	0.76 ₀₂	0.74 ₀₃	0.87 ₀₁	0.93 ₀₁	0.63 ₀₃	0.83 ₀₃	0.92 ₀₃	0.82 ₀₀	0.81 ₀₀
	TabPFN	0.91 ₀₀	0.74 ₀₃	0.94 ₀₀	1.00 ₀₀	0.75 ₀₃	0.81 ₀₃	0.92 ₀₂	0.89 ₀₀	0.93 ₀₀
	TabLLM	0.92 ₀₀	0.70 ₀₄	0.96 ₀₀	1.00 ₀₀	0.70 ₀₂	0.80 ₀₄	0.94 ₀₁	0.92 ₀₀	1.00 ₀₀
	LLaMA	0.94 ₀₀	0.72 ₀₄	0.97 ₀₀	1.00 ₀₀	0.76 ₀₇	0.84 ₀₃	0.93 ₀₁	0.93 ₀₀	1.00 ₀₀
	LLaMA-GTL	0.94 ₀₀	0.75 ₀₅	0.96 ₀₀	1.00 ₀₀	0.76 ₀₆	0.85 ₀₄	0.93 ₀₁	0.93 ₀₀	1.00 ₀₀