NANYANG TECHNOLOGICAL UNIVERSITY

SIGMOD
PODS
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Machine Learning for Databases: Foundations, Paradigms, and Open problems

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Machine Learning for Databases (ML4DB)

- Machine learning techniques have been used to improve various aspects of a data management system
  - Core components: index, data layout, query optimizer, scheduler…
  - Advisors: knob tuning, index/view advisor, performance prediction…
  - Usability: text2SQL

- Existing tutorials on ML4DB
  - Survey ML solutions for different database problems
  - Focus on ML solutions for a particular problem

Tutorial Overview

- ML4DB Foundations (1 hour 15 mins)
  What are the key components for foundation in ML4DB?
- ML4DB Paradigms (1 hour 15 mins)
  “Replacement” approach vs. “ML-enhanced” approach
- ML4DB Open problems (30 mins)
  What are the open problems to be solved?

Tutorial Overview

- ML4DB Foundations
  - Query Plan Representation
  - Pretrained Models
- ML4DB Paradigms
  - Replace vs Enhance
  - Learned Index
  - Learned Optimizer
- ML4DB Open problems
  - What are the foundations of ML4DB?
  - Model efficiency
  - Generating training data of high quality
  - Handling data & workload shifts
  - Foundation models (Pretrained models) for Ml4DB
  - LLMs for ML4DB

ML4DB Foundations

- Can we have some foundations that are relevant to different ML4DB systems?

- We identify two key foundations
  - Query plan representation
  - Pretrained models

ML4DB Foundations

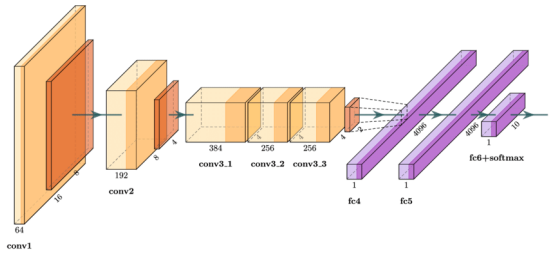
- Can we have some foundations that are relevant to different ML4DB systems?

- We identify two key foundations
  - Query plan representation
  - Pretrained models

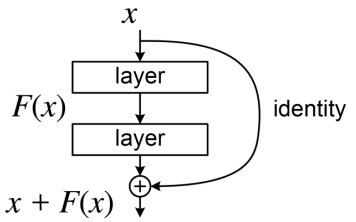
Foundations in other domains

- **Computer Vision**: as **input representation techniques** improve, all task performances get better.

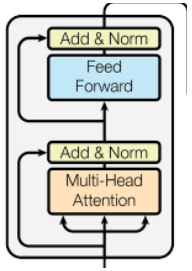
Input representation techniques



AlexNet (2012)



ResNet (2015)



Vision Transformer (2020)

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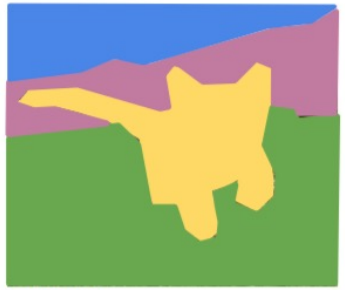
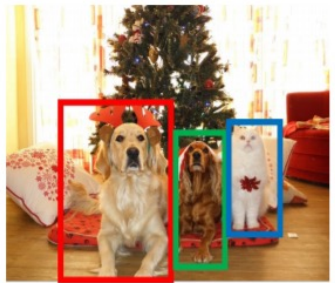
Apply to

Computer vision tasks

Classification



Semantic Segmentation



Object Detection

Instance Segmentation

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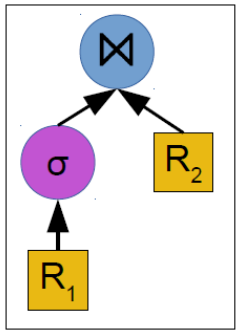
Picture from http://cs231n.Stanford.edu/slides/2020/lecture_12.pdf

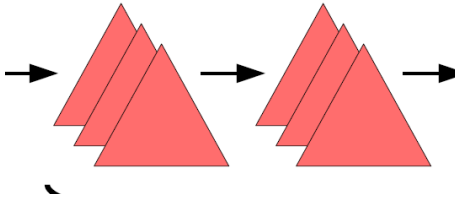
ML4DB Analogy

- Query plan representation techniques can be applied to various database tasks

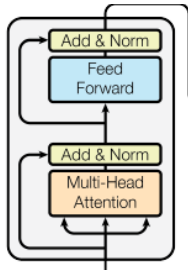
Query plan representation techniques



QPPNet



TreeCNN



Transformers

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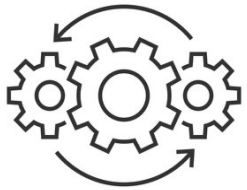
Apply to

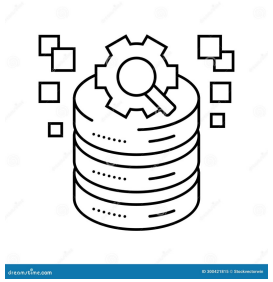
Database tasks

Index Tuner

Cost Estimator



View advisor



Optimizer

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Physical query plans

- A query plan is a sequence of steps used to access data in a relational database management system.

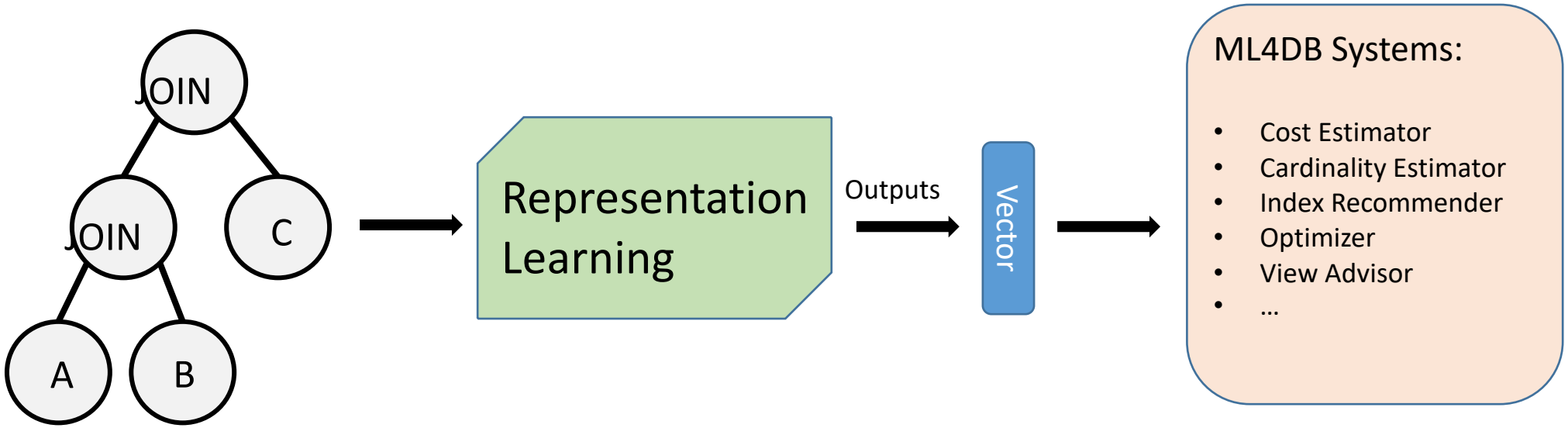
```
EXPLAIN SELECT *
FROM tenk1 t1, tenk t2
WHERE t1.unique1 < 100 AND
t1.unique2 = t2.unique2;
```

```
Merge Join  (cost=198.11..268.19 rows=10 width=488)
  Merge Cond: (t1.unique2 = t2.unique2)
  ->  Index Scan using tenk1_unique2 on tenk1 t1  (cost=0.29..656.28 rows=101 width=244)
        Filter: (unique1 < 100)
  ->  Sort  (cost=197.83..200.33 rows=1000 width=244)
        Sort Key: t2.unique2
        ->  Seq Scan on tenk t2  (cost=0.00..148.00 rows=1000 width=244)
```

Query plan from Postgres. https://www.postgresql.org/docs/current/using-explain.html.

Query Plan Representation

- **Query Plans** are used as inputs in many ML4DB systems
- **Query plan representation** is a key operation
- Research Problem: Given a *query plan*, learn a vector representation to be used as the input to a ML4DB system

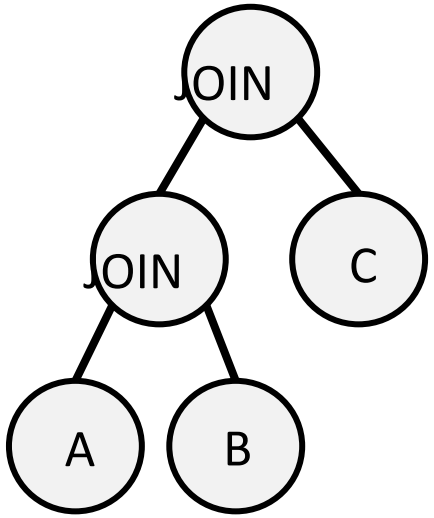


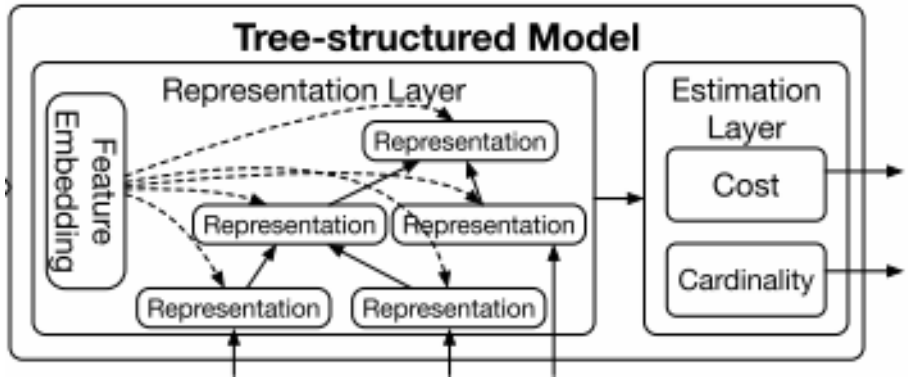
Zhao Y, et al. QueryFormer: a tree transformer model for query plan representation. VLDB 2022.

Example: Cost Estimation

- Cost and Cardinality Estimation
  - Uses Tree-LSTM to extract feature representation from a *query plan*
  - Uses MLP to predict cost and cardinality

Model Input





Model Output

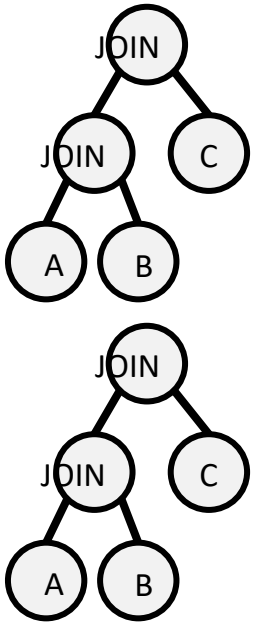
Est. Cost: 123 ms
Est. Cardinality: 12345

Ji Sun, Guoliang Li. An End-to-End Learning-based Cost Estimator. VLDB 2019.

Example: Index Recommendation

- Index Recommendation
  - Featurize a *query plan* by creating feature channels for each physical operator
  - Perform classification on *query plan* pairs

Model Input



Seek_Row_Serial	10
Scan_Row_Serial	80
HJ_Row_Serial	55
NLJ_Row_Serial	0
MJ_Row_Serial	0
...	...

Seek_Row_Serial	30
Scan_Row_Serial	30
HJ_Row_Serial	55
NLJ_Row_Serial	0
MJ_Row_Serial	0
...	...

EstNodeCost (P_1)

EstNodeCost ($P_2 - P_1$)

Seek_Row_Serial	20
Scan_Row_Serial	-50
HJ_Row_Serial	0
NLJ_Row_Serial	0
MJ_Row_Serial	0
...	...

EstNodeCost (P_2)

Seek_Row_Serial	200
Scan_Row_Serial	2000
HJ_Row_Serial	4600
NLJ_Row_Serial	0
MJ_Row_Serial	0
...	...

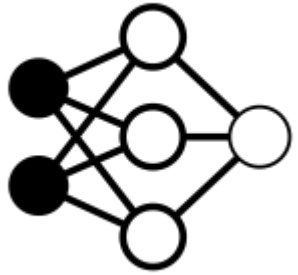
Seek_Row_Serial	1200
Scan_Row_Serial	1000
HJ_Row_Serial	6200
NLJ_Row_Serial	0
MJ_Row_Serial	0
...	...

LeafWeightEst RowsWeighted Sum (P_1)

LeafWeightEstRows WeightedSum (P_2 - P_1)

Seek_Row_Serial	1000
Scan_Row_Serial	-1000
HJ_Row_Serial	1600
NLJ_Row_Serial	0
MJ_Row_Serial	0
...	...

LeafWeightEst RowsWeighted Sum (P_2)



Classifier

Model Output

First plan is better

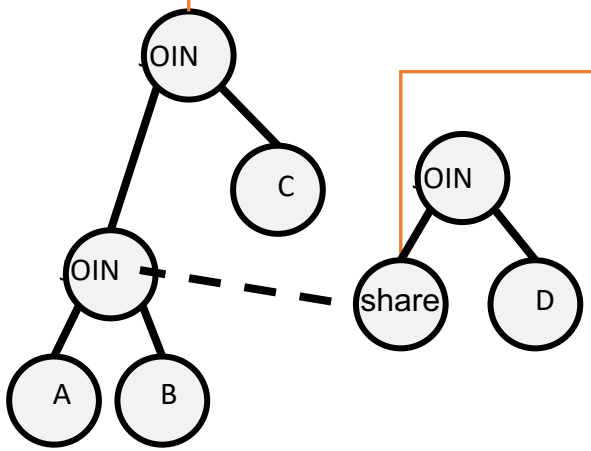
First index is better

Ding, B, et al. AI Meets AI: Leveraging Query Executions to Improve Index Recommendations. Sigmod 2019.

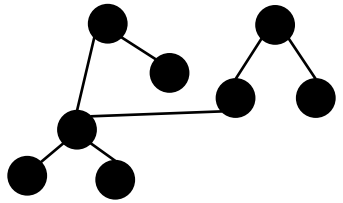
Example： Concurrent query optimization

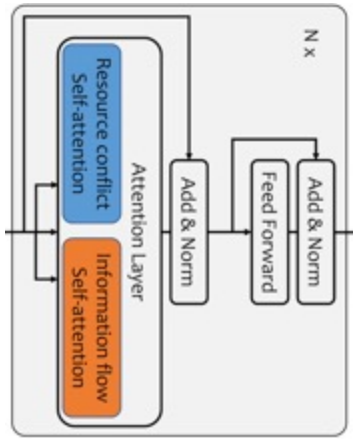
- Concurrent query optimization
  - Featurize *multiple (partial) query plans*
  - Featurize *SQL query* by extracting join graph and predicate information
  - Predict the cost for plan generation

Model Input



Join	Scan	Share	A	B	…
1	0	0	1	1	…
0	0	1	1	1	…
…	…	…	…	…	…





Cost estimation model

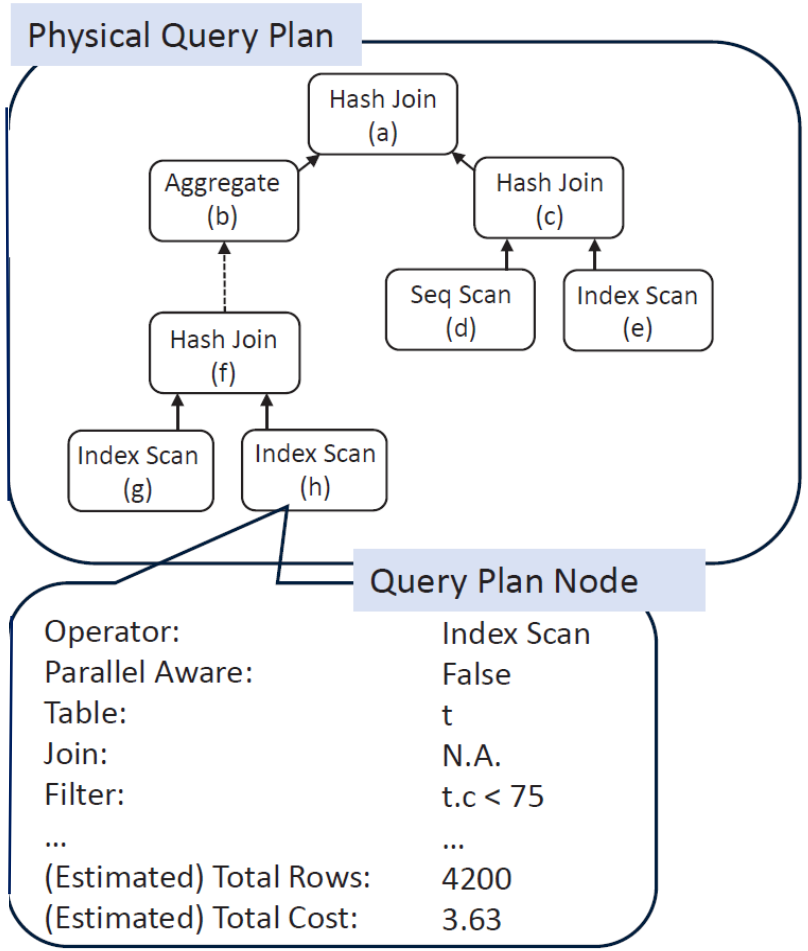
Model Output

cost

Mo, S, et al. Lemo: A Cache-Enhanced Learned Optimizer for Concurrent Queries. SIGMOD 2024

Query Plan Representation as a Foundation

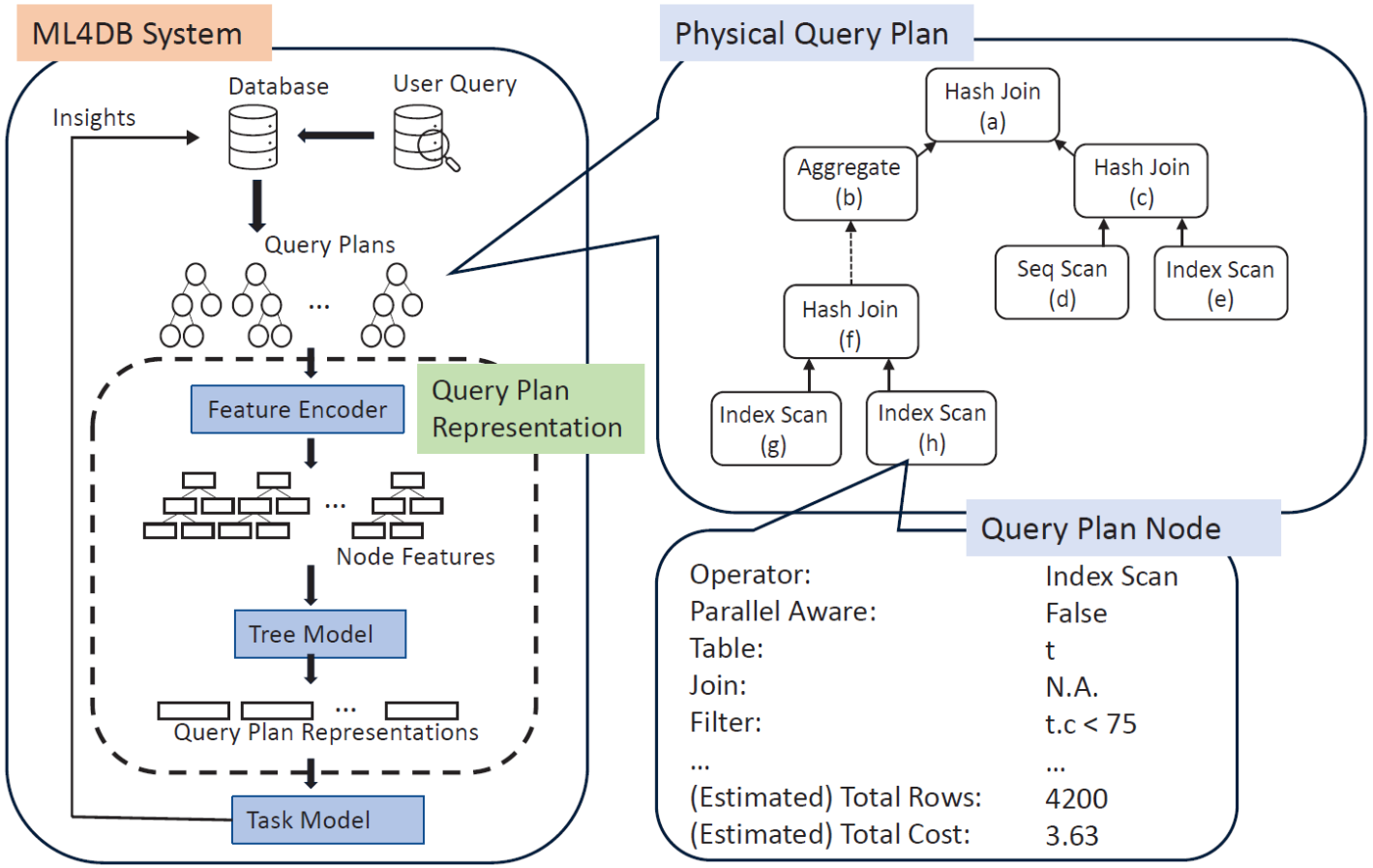
- Why is representation learning important?
  - Non-trivial to define features from a query plan
  - Difficult to deal with the tree structure of a query plan
  - A key factor to the performance of all these tasks



Zhao, Y, et al. A Comparative Study and Component Analysis of Query Plan Representation Techniques in ML4DB Studies. VLDB 2024.

Query Plan Representation in ML4DB Pipeline

- Can be broadly broken down to two components
  - Feature Encoder
  - Tree Model



Zhao, Y, et al. A Comparative Study and Component Analysis of Query Plan Representation Techniques in ML4DB Studies. VLDB 2024.

Query Plan Representation in ML4DB Pipeline

- Tree Models: *LSTM, TreeCNN, Transformer, TreeLSTM*, etc.
- Feature Encoding: *Operator, Predicate, Table*, Various *Database statistics*.

A summary of query plan representation methods and their components.

Method	Original Task	Tree Model	Encoding Information			
			Operator	Table	Predicate	Database Statistics
AVGDL [51]	View Selection	LSTM	Yes	Yes	Yes	-
AIMeetsAI [8]	Index Selection	Feature Vector	Yes	-	-	Estimates
ReJOIN [30]	Join Order Selection	Feature Vector	Yes	Yes	Column	-
BAO [28]	Optimizer	TreeCNN	Yes	-	-	Estimates
NEO [29]	Optimizer	TreeCNN	Yes	Yes	Column	Estimates
Prestroid [17]	Cost Estimation	TreeCNN	Yes	Yes	Yes	-
E2E-Cost [39]	Cost/Card Estimation	TreeLSTM	Yes	Yes	Yes	Sample
RTOS [50]	Join Order Selection	TreeLSTM	Yes	Yes	Yes	-
Plan-Cost [31]	Cost Estimation	TreeRNN	Yes	-	-	Estimates
QueryFormer [54]	General Purpose	Transformer	Yes	Yes	Yes	Sample & Histogram

Zhao, Y, et al. A Comparative Study and Component Analysis of Query Plan Representation Techniques in ML4DB Studies. VLDB 2024.

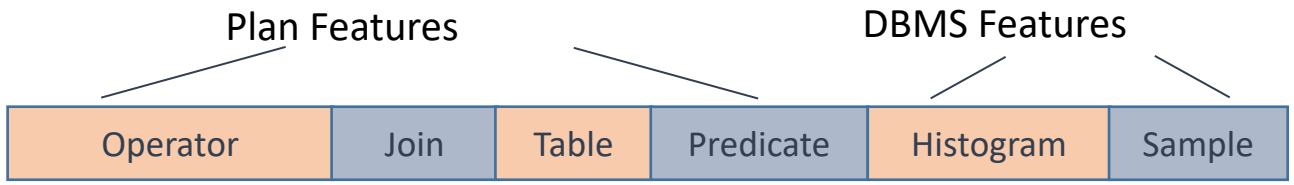
Feature Encoding

- Challenge:
  - How to select features to encode from a query plan node?

	Content	Example	Encoding
Plan Features	Operator	hash scan	One-hot / Embedding
	Table	title as t	One-hot / Embedding
	Column	t.production_year	One-hot / Embedding
	Predicate	t.production_year > 1965	<col, op, val> triplet
	Join	t.id = mc.movie_id	One-hot / Embedding
DBMS enhanced	Database Estimates	est. Rows: 400	Normalized value
	Samples	[1,0,0,0,1,0,0,1,0]	Bitmap
	Histogram	[0, 0, 0, 0, 0, 0, 1, 1, 1]	Bitmap/ Normalized value
	…	…	…

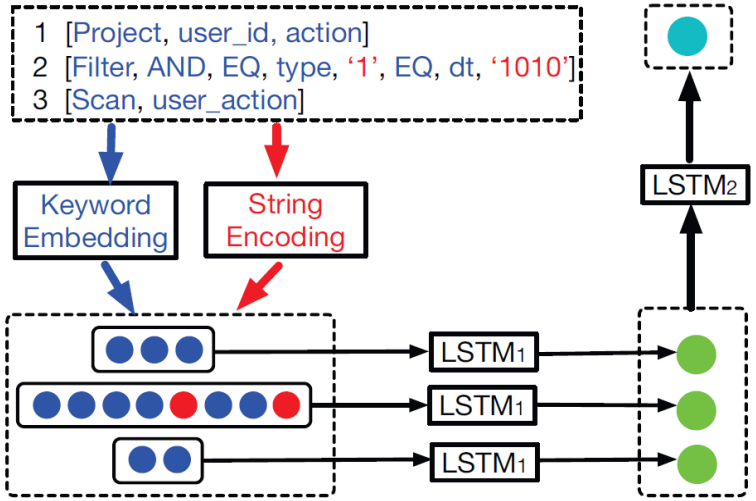
Feature Encoding

- How to combine the features?
  - Concatenate the features (most Popular)



  - Feature Channels [Ding, B, et al. SIGMOD 19]

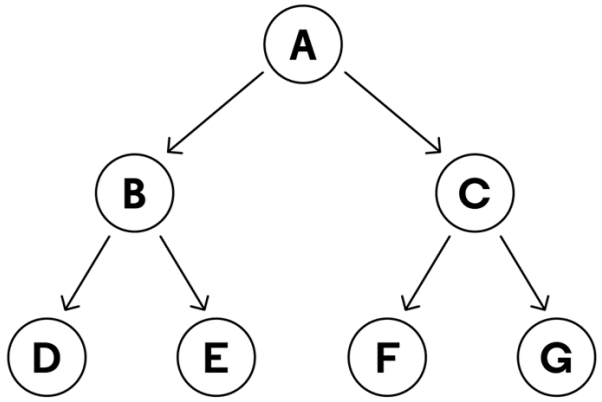
Seek_Row_Serial	10
Scan_Row_Serial	80
HJ_Row_Serial	55
NLJ_Row_Serial	0
MJ_Row_Serial	0
...	...

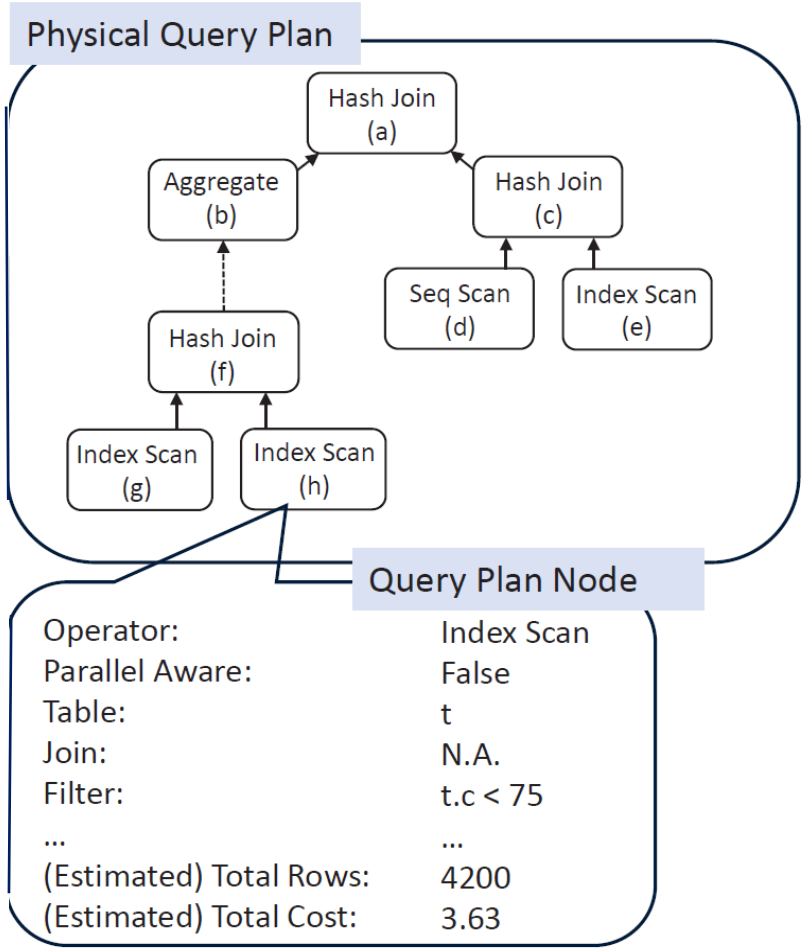


  - Deep Learning Models, i.e., LSTM, to join the encoded components [Yuan, H, et al. ICDE 2020]

Tree Models

- How to handle the tree structure of query plans?
  - Directional dependence
  - Irregular shapes

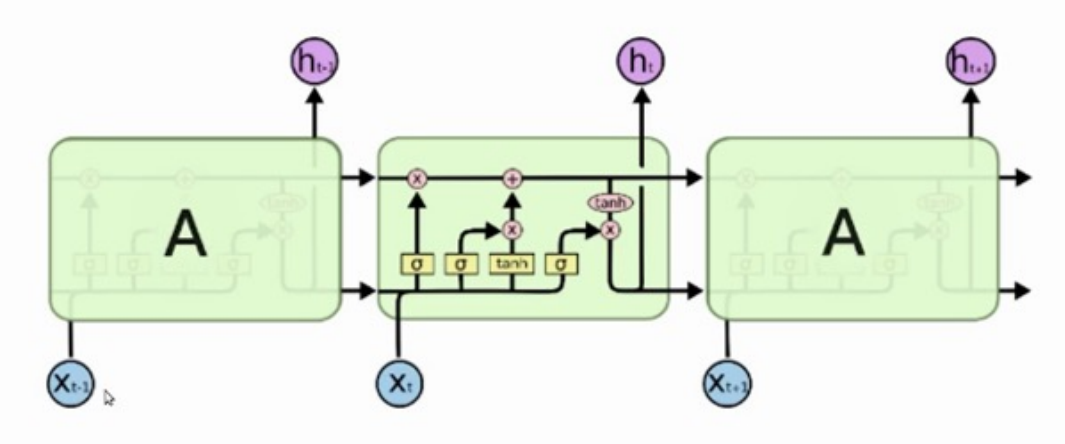




Flat sequence model, e.g., LSTM

- LSTM
  - Using gates to solve ‘gradient vanishing’ and ‘gradient explosion’

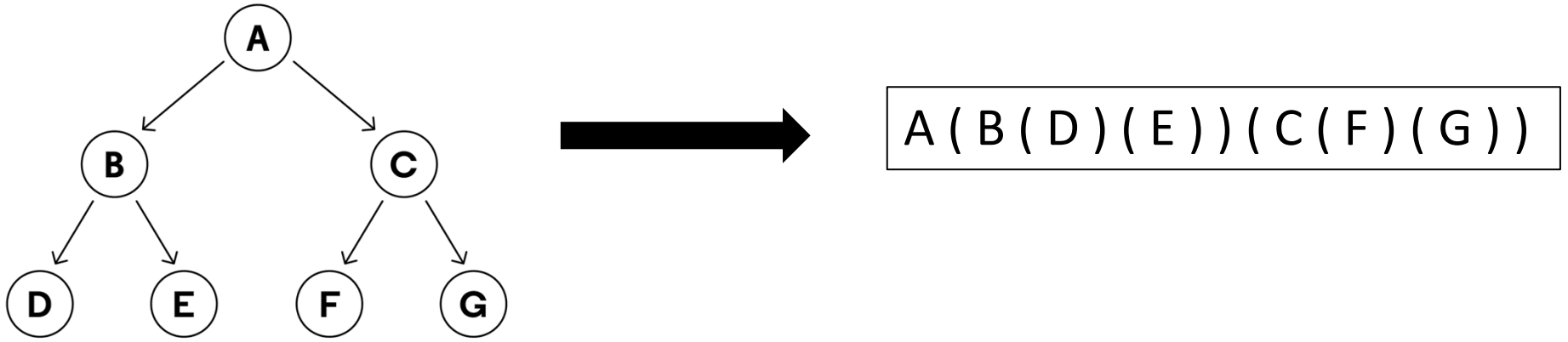
$$
\begin{aligned}
i_t &= \sigma\left(W^{(i)}x_t + U^{(i)}h_{t-1} + b^{(i)}\right), \\
f_t &= \sigma\left(W^{(f)}x_t + U^{(f)}h_{t-1} + b^{(f)}\right), \\
o_t &= \sigma\left(W^{(o)}x_t + U^{(o)}h_{t-1} + b^{(o)}\right), \\
u_t &= \tanh\left(W^{(u)}x_t + U^{(u)}h_{t-1} + b^{(u)}\right), \\
c_t &= i_t \odot u_t + f_t \odot c_{t-1}, \\
h_t &= o_t \odot \tanh(c_t),
\end{aligned}
$$



Hochreiter, S and Schmidhuber J. Long Short-Term Memory (LSTM). Neural Computation 1995.

Flat sequence model, e.g., LSTM

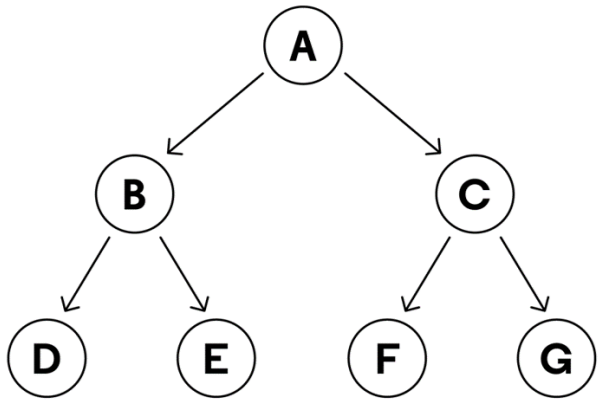
- Step 1: DFS to convert the tree to sequence
- Step 2: Apply LSTM to obtain output representation



Hochreiter, S and Schmidhuber J. Long Short-Term Memory (LSTM). Neural Computation 1995.

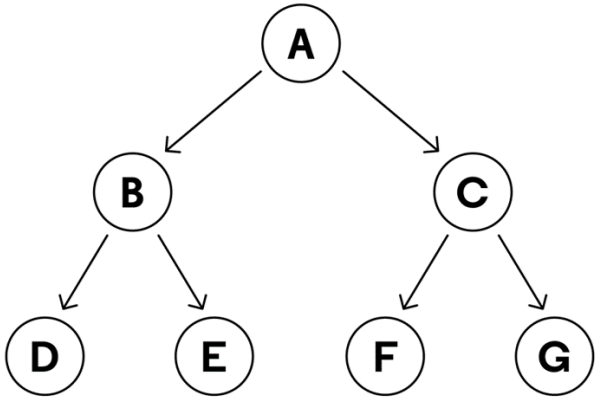
Tree RNN

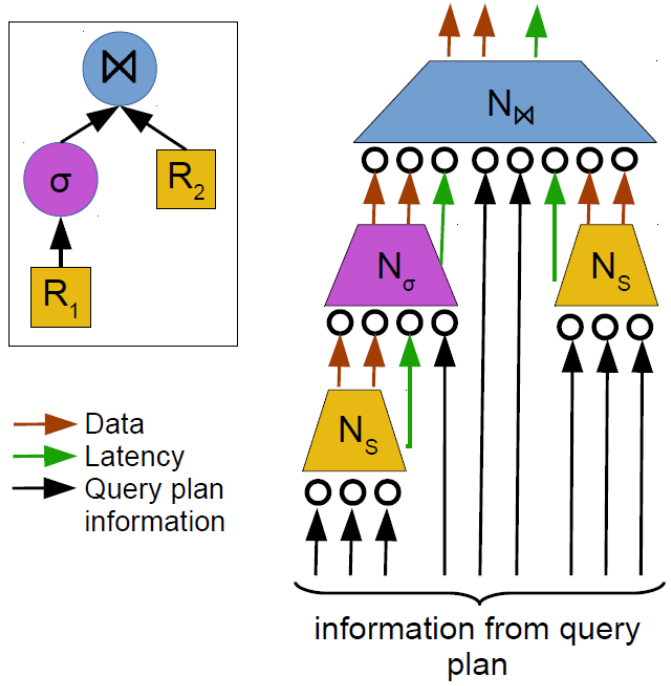
- Can we pass information bottom-up, just like how a query plan is processed?



Tree RNN

- Can we pass information bottom-up, just like how a query plan is processed?
  - Tree Structured RNN model
  - Pass the information regardless of tree shape

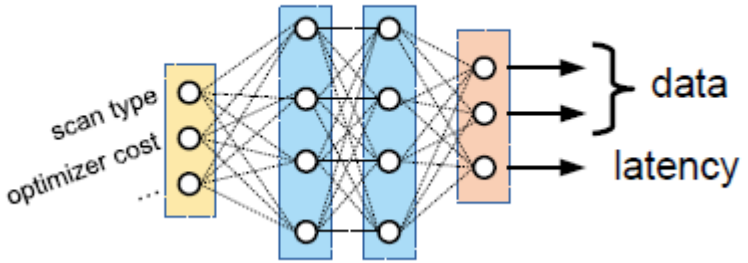


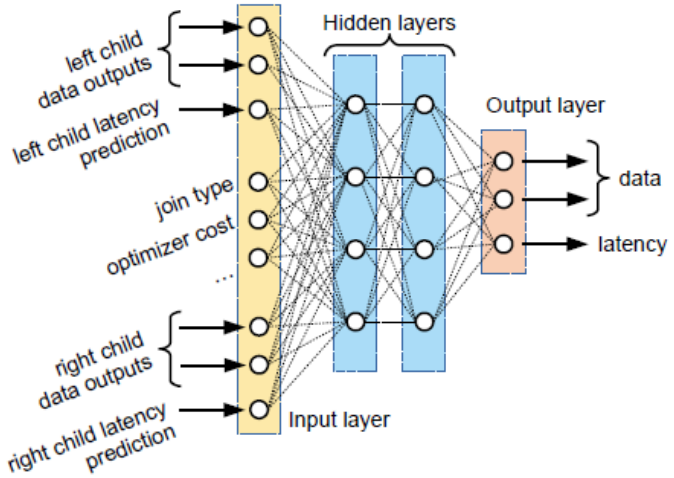


Ryan Marcus, Olga Papaemmanouil. Plan-Structured Deep Neural Network Models for Query Performance Prediction. VLDB 2019.

Tree RNN

- Two novel neural units:
  - Scan
  - Join





- How to perform batching?
  - Group query plans of the same shape

Ryan Marcus, Olga Papaemmanouil. Plan-Structured Deep Neural Network Models for Query Performance Prediction. VLDB 2019.

Tree LSTM

- Can we apply some advanced ML technique to Tree RNN setup?

Tree LSTM

- Can we apply some advanced ML technique to Tree RNN setup?
  - Use LSTM-cell at each step
  - First explored in NLP
  - Child-sum vs N-ary Tree LSTM

$$\hat{h}_j = \sum_{k \in C(j)} h_k$$

$$i_j = \sigma(W^{(i)} x_j + U^{(i)} \hat{h}_j + b^{(i)})$$

$$f_{jk} = \sigma(W^{(f)} x_j + U^{(f)} h_k + b^{(f)})$$

$$o_j = \sigma(W^{(o)} x_j + U^{(o)} \hat{h}_j + b^{(o)})$$

$$u_j = \tanh(W^{(u)} x_j + U^{(u)} \hat{h}_j + b^{(u)})$$

$$C_j = i_j \odot u_j + \sum_{k \in C(j)} f_{jk} \odot c_k$$

$$h_j = o_j \odot \tanh(c_j)$$

$$i_j = \sigma\left(W^{(i)} x_j + \sum_{\ell=1}^{N} U_\ell^{(i)} h_{j\ell} + b^{(i)}\right),$$

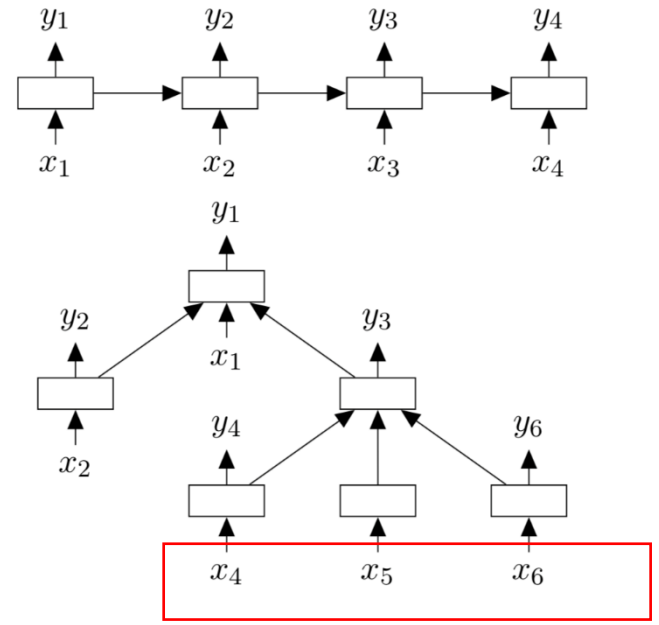
$$f_{jk} = \sigma\left(W^{(f)} x_j + \sum_{\ell=1}^{N} U_{k\ell}^{(f)} h_{j\ell} + b^{(f)}\right),$$

$$o_j = \sigma\left(W^{(o)} x_j + \sum_{\ell=1}^{N} U_\ell^{(o)} h_{j\ell} + b^{(o)}\right),$$

$$u_j = \tanh\left(W^{(u)} x_j + \sum_{\ell=1}^{N} U_\ell^{(u)} h_{j\ell} + b^{(u)}\right),$$

$$c_j = i_j \odot u_j + \sum_{\ell=1}^{N} f_{j\ell} \odot c_{j\ell},$$

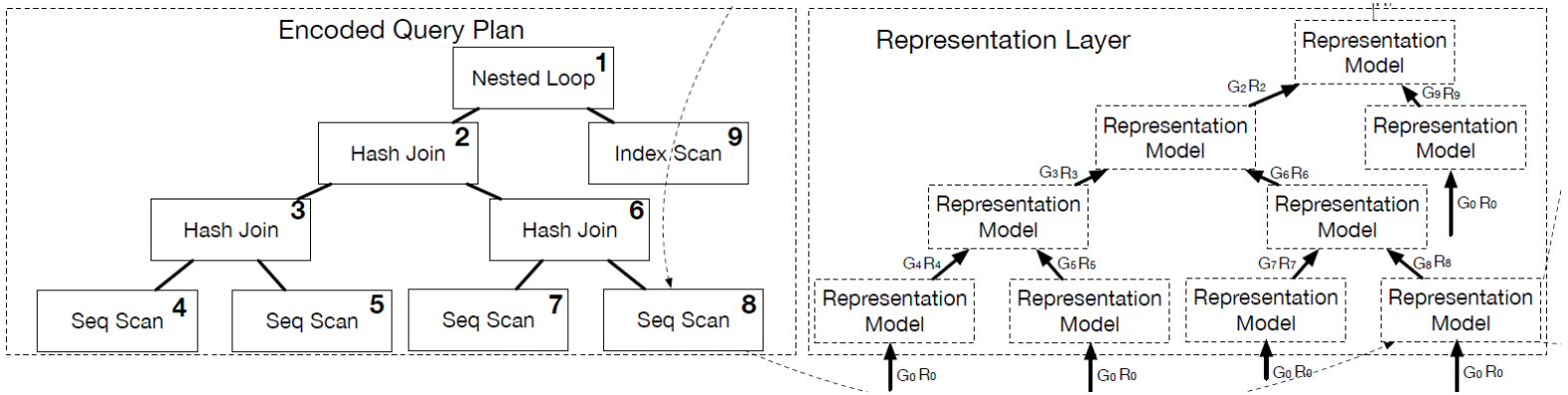
$$h_j = o_j \odot \tanh(c_j),$$



Tai, K S, et, al. Improved Semantic Representations From Tree-Structured Long Short-Term Memory Networks. ACL 2015.

Tree LSTM

- Apply Tree LSTM to query plan representation
  - Traverse the tree bottom up
  - Apply the LSTM cell at each step

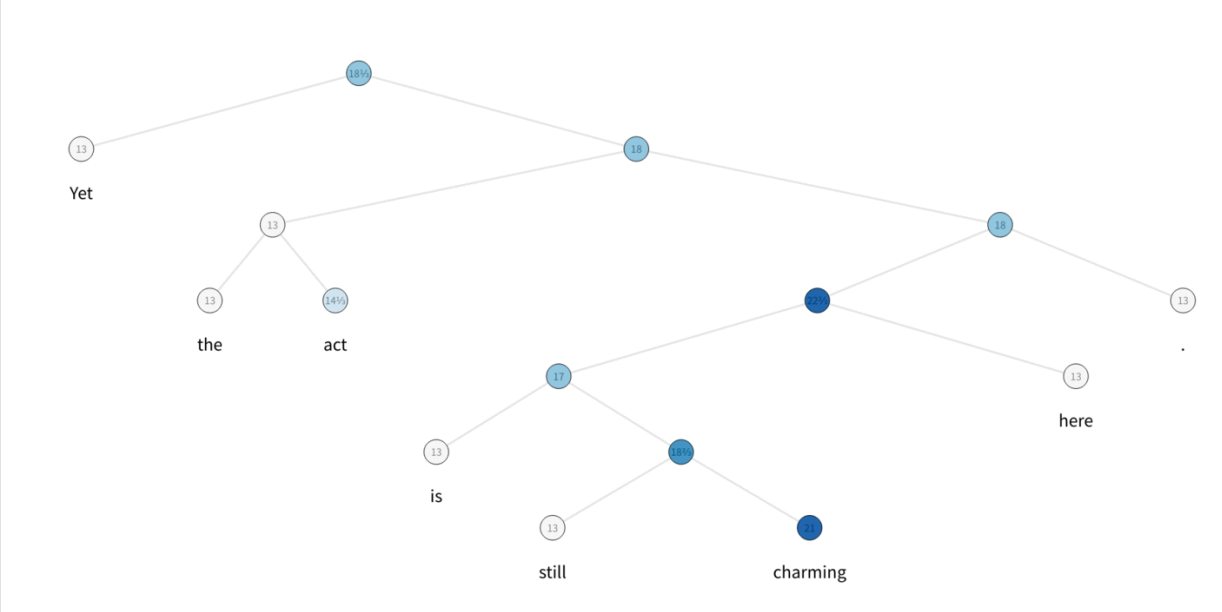


- How do we do batching now?

Ji Sun, Guoliang Li. An End-to-End Learning-based Cost Estimator. VLDB 2019.

Tree LSTM Batching

- Parent Node depends on children node results
  - Assign 'height' of nodes to the forest (batch of query plan trees)
  - Process nodes with height=0 (scan nodes)
  - Process nodes with height=1
  - ..

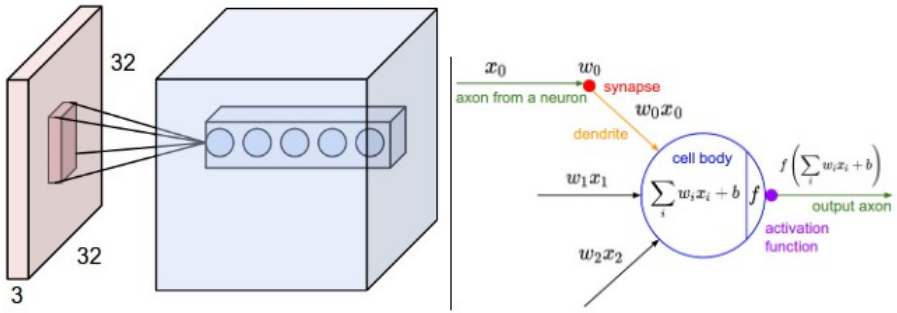


Picture from dgl documentation. https://docs.dgl.ai/tutorials/models/2_small_graph/3_tree-lstm.html

Ji Sun, Guoliang Li. An End-to-End Learning-based Cost Estimator. VLDB 2019.

Tree CNN

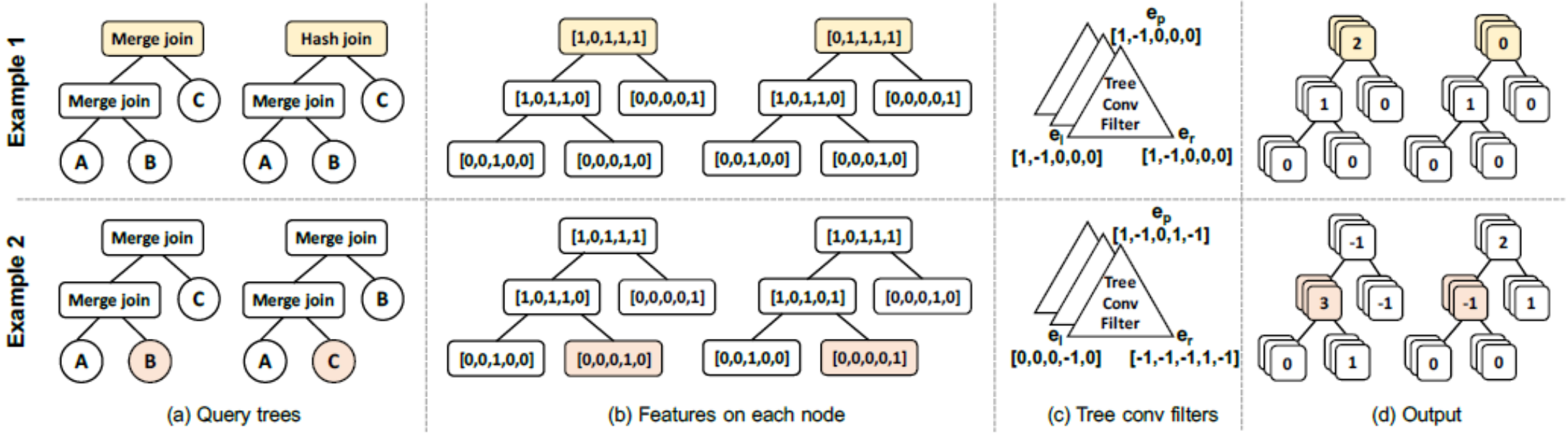
- Idea:
  - An extension to traditional CNN
  - Conv layers as pattern matching
    - Image: edges, shapes, etc.,
    - Query plans: nest loop over index scan, etc.,



Picture from https://cs231n.github.io/convolutional-networks/

Tree CNN

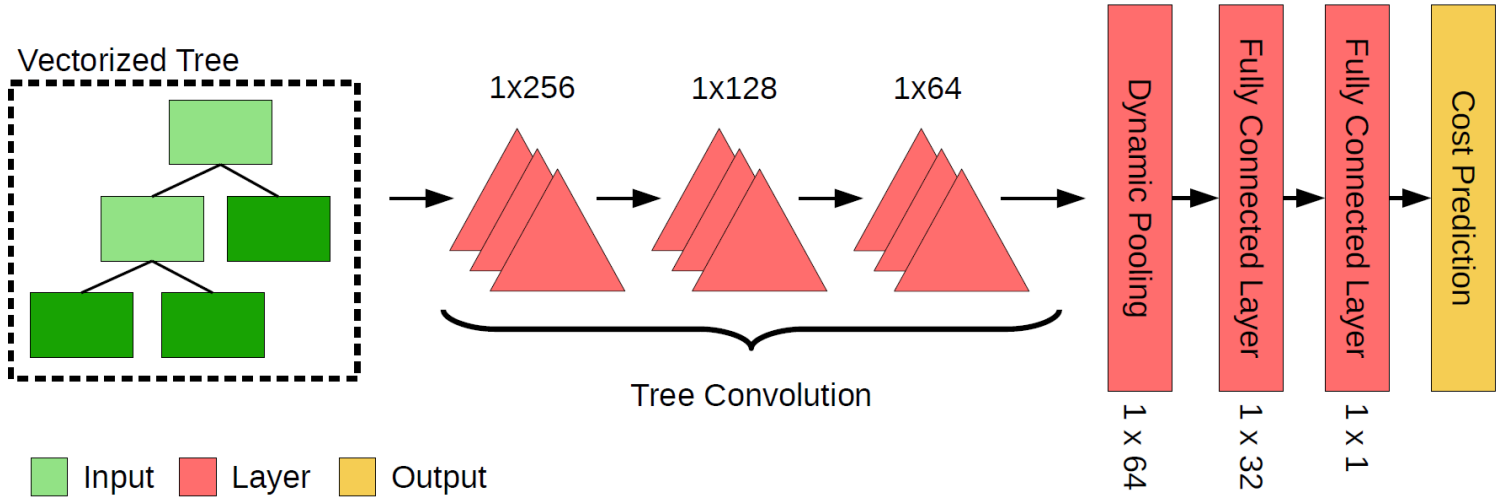
- Idea:
  - Triangular-shape (parent-child-child) convolution filters
  - ‘Slide’ over a query plan tree to match patterns, just like CNN to image



Marcus, R, et al. Neo: A Learned Query Optimizer. VLDB 2019.

Tree CNN

- Network Architecture
  - Stack of Tree Conv layers
  - Dynamic Pooling to unify output size

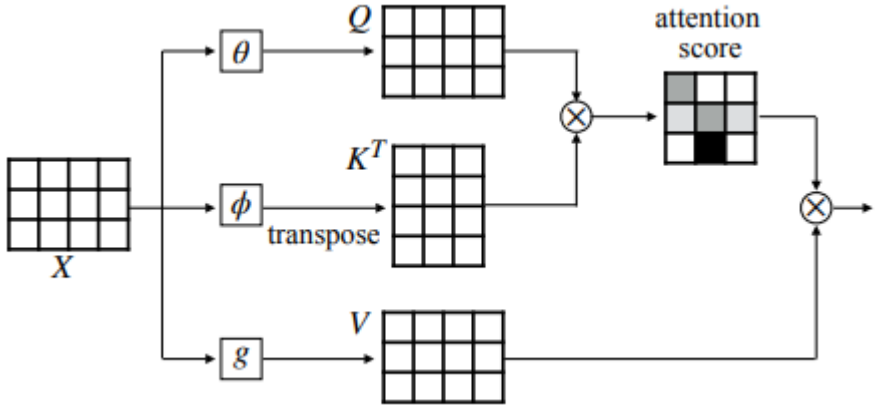


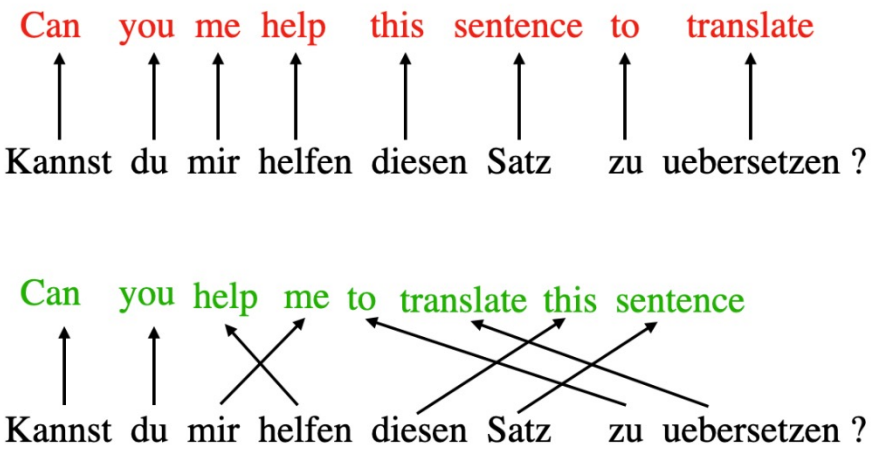
Marcus, R, et al. Neo: A Learned Query Optimizer. VLDB 2019.

Transformers

- Attention mechanism
  - To capture pair-wise dependency and interaction among elements

$$Attention(Q, K, V) = softmax(\frac{QK^T}{\sqrt{d_k}})V,$$

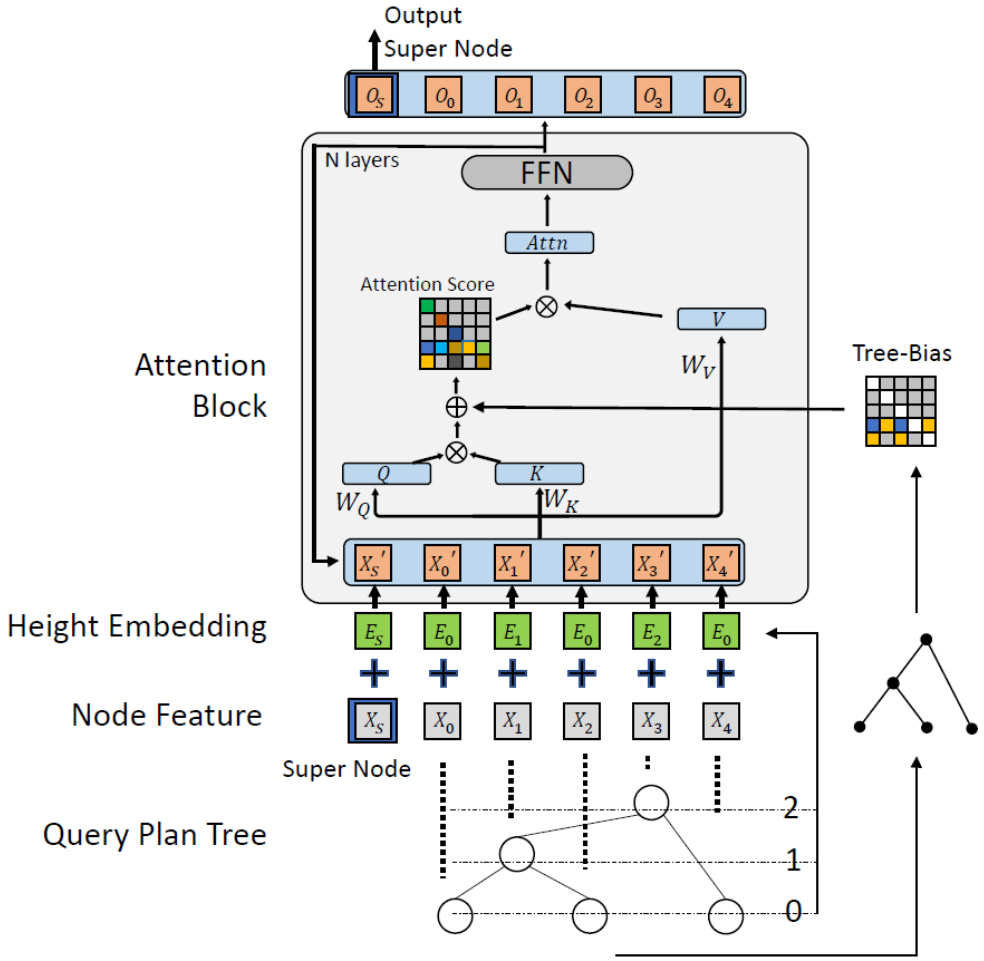




Picture from https://blogs.oracle.com/ai-and-datascience/post/multi-head-self-attention-in-nlp

QueryFormer

- Challenge
  - How to infuse the tree structure?
- Solution: Tree-biased attention
  - Bias the attention score by path distance d, specifically:
  - Contribution of j to node i: $A_{ij} = \frac{Q_i K_j^T}{\sqrt{d_k}}$
  - New attention: $A'_{ij} = A_{ij} + b_d$, where b_d is a learnable scalar, d is distance between i and j



Zhao, Y, et al, QueryFormer: a tree transformer model for query plan representation. VLDB 2022.

Summary

- A representation method: a combination of **tree model** and **feature encoding**.

A summary of query plan representation methods and their components.

Method	Original Task	Tree Model	Encoding Information			
			Operator	Table	Predicate	Database Statistics
AVGDL [51]	View Selection	LSTM	Yes	Yes	Yes	-
AIMeetsAI [8]	Index Selection	Feature Vector	Yes	-	-	Estimates
ReJOIN [30]	Join Order Selection	Feature Vector	Yes	Yes	Column	-
BAO [28]	Optimizer	TreeCNN	Yes	-	-	Estimates
NEO [29]	Optimizer	TreeCNN	Yes	Yes	Column	Estimates
Prestroid [17]	Cost Estimation	TreeCNN	Yes	Yes	Yes	-
E2E-Cost [39]	Cost/Card Estimation	TreeLSTM	Yes	Yes	Yes	Sample
RTOS [50]	Join Order Selection	TreeLSTM	Yes	Yes	Yes	-
Plan-Cost [31]	Cost Estimation	TreeRNN	Yes	-	-	Estimates
QueryFormer [54]	General Purpose	Transformer	Yes	Yes	Yes	Sample & Histogram

Zhao Y, et al, A Comparative Study and Component Analysis of Query Plan Representation Techniques in ML4DB Studies. VLDB 2024.

What to evaluate and how?

- Open Problems:
  - Are query plan representation methods interchangeable across tasks?
  - What is the best tree model design?
  - What is the best feature encoding?
- Experimental Methodology:
  - Interchange and compare query plan representation methods in 3 ML4DB systems
  - Fix feature encoding and compare tree models
  - Fix tree model and compare feature encoding

Zhao Y, et al, A Comparative Study and Component Analysis of Query Plan Representation Techniques in ML4DB Studies. VLDB 2024.

Experimental Settings

- Methodology:
  - Perform database tasks by replacing **query plan representation** of ML4DB systems.
    - Cost Estimation
    - Index Selection
    - (Steer) Query Optimizer
- Dataset: both synthetic and real workloads with different characteristics

Query Plan Sizes in datasets.

Dataset	Max #	Avg #	Skewness	Correlation
TPC-H	26	16.8	Uniform	Uncorrelated
TPC-DS	143	44.4	Uniform	Uncorrelated
Synthetic	10	4.9	Moderate	Moderate
JOB-Light	14	8.44	Moderate	Moderate
STATS	16	9.49	High	High
Job-Extend	73	21.2	Moderate	Moderate

Zhao Y, et al, A Comparative Study and Component Analysis of Query Plan Representation Techniques in ML4DB Studies. VLDB 2024.

Key Finding 1

Are query plan representation methods interchangeable across tasks?

- Yes. QueryFormer and BAO performs well across tasks.

Query Plan Representation Across Tasks

Method/ Component	Cost (ID)	Cost (OOD)	Index (ID)	Index (OOD)	Optimizer
AVGDL	++	-	++	-	++
AIMEETSAI	++	-	+	-	-
ReJOIN	-	-	-	+	- -
BAO	++	++	++	+	+
NEO	-	+	+	+	-
Prestroid	-	+	+	-	+
E2E-Cost	++	+	-	-	- -
RTOS	++	-	+	+	+
Plan-Cost	+	-	-	-	-
QueryFormer	++	++	++	+	+

Zhao Y, et al, A Comparative Study and Component Analysis of Query Plan Representation Techniques in ML4DB Studies. VLDB 2024.

Key Finding 2

What is the best tree model design?

- Surprisingly, tree model is **less** important when fixing feature encoding
  - It does not matter in cost estimation
  - When relative ranking matters (in index selection and optimization)
    - TreeCNN works best for in-distribution workload
    - LSTM works best for out-of-distribution workload

Table 4: Tree Model Comparison

Method/ Component	Cost (ID)	Cost (OOD)	Index (ID)	Index (OOD)	Optimizer
TreeCNN	++	+	++	+	+
TreeLSTM	++	+	+	-	-
LSTM	++	+	+	++	++
Transformer	++	+	+	+	-

Zhao Y, et al, A Comparative Study and Component Analysis of Query Plan Representation Techniques in ML4DB Studies. VLDB 2024.

Key Finding 3

What is the best feature encoding?

- *Database Estimate* is the most effective feature
- Despite individual feature effectiveness, different encoding strategies should be adopted depending on task requirement
  - To optimize **absolute error** (cost estimation), concatenate as much feature as possible
  - To optimize **relative ranking** (index selection, optimization), *Database Estimate* and *Histogram* are the best features

Table 5: Feature Encoding Comparison

Method/ Component	Cost (ID)	Cost (OOD)	Index (ID)	Index (OOD)	Optimizer
Pred	++	+	-	+	+
Est	++	+	++	++	++
Hist	-	-	+	+	++
Sample	+	-	+	-	-

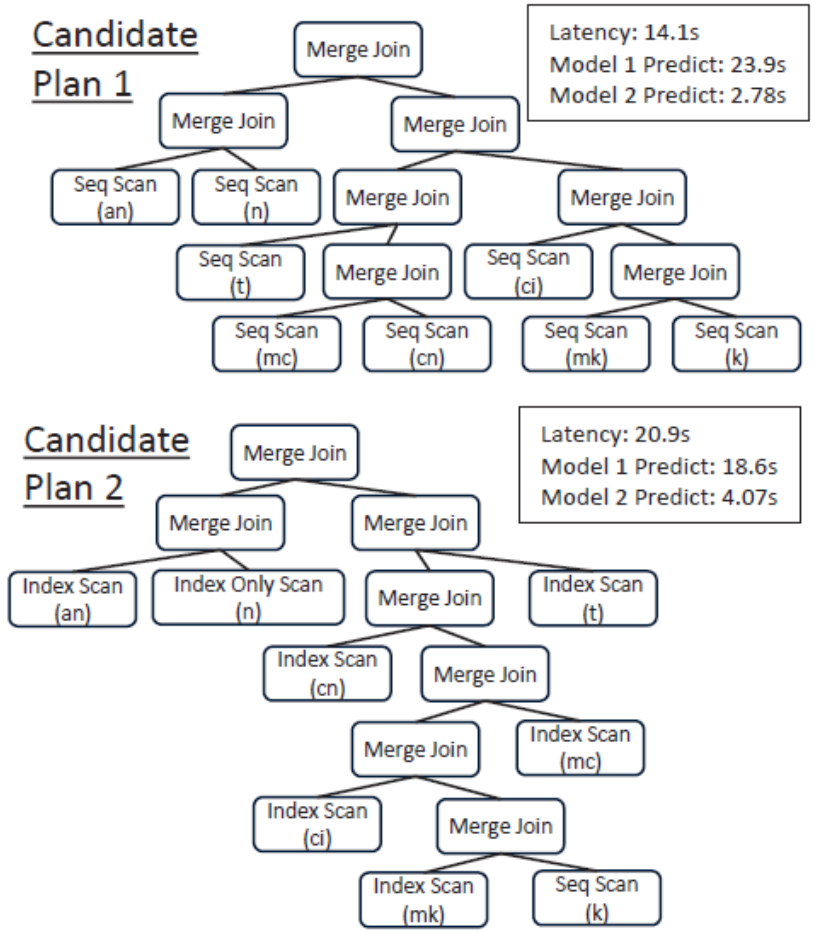
Zhao Y, et al, A Comparative Study and Component Analysis of Query Plan Representation Techniques in ML4DB Studies. VLDB 2024.

Why relative ranking differ from cost estimation?

- Case Study
  - Higher absolute accuracy does not guarantee better distinguishing power

QUERY

```
SELECT
  MIN(an.name) AS cool_actor,
  MIN(t.title) AS series_named
FROM
  aka_name AS an,
  cast_info AS ci,
  company_name AS cn,
  keyword AS k,
  movie_companies AS mc,
  movie_keyword AS mk,
  name AS n,
  title AS t
WHERE
  cn.country_code ='[us]' AND
  k.keyword ='character' AND
  t.episode_nr < 100 AND
  an.person_id = n.id AND
  n.id = ci.person_id AND
  ci.movie_id = t.id AND
  t.id = mk.movie_id AND
  mk.keyword_id = k.id AND
  t.id = mc.movie_id AND
  mc.company_id = cn.id AND
  an.person_id = ci.person_id AND
  ci.movie_id = mc.movie_id AND
  ci.movie_id = mk.movie_id AND
  mc.movie_id = mk.movie_id;
```



Zhao Y, et al, A Comparative Study and Component Analysis of Query Plan Representation Techniques in ML4DB Studies. VLDB 2024.

Take-aways for Query Plan Representation

- Query plan representation consists of **feature encoding** and **tree models**
- The optimal design should be selected based on task requirements
  - Feature encoding
    - *Histogram, Database Estimate* for relative rankings
    - The more the better for absolute numbers
  - Tree models
    - TreeCNN works best for in-distribution workload
    - LSTM works best for out-of-distribution workload

ML4DB Foundations

- Can we have some foundations that are relevant to different ML4DB systems?

- We identify two key foundations
  - Query plan representation
  - Pretrained models

Analogy to other domains

- LLMs: pretrained on large and diverse corpora

Chatbot, translation, text summarization, classification, etc., or as **zero-shot models**

Fine-tune/
RAG, etc.

Legal document analysis, customer support, technical document assistance, etc., or as **base models**

Analogy to other domains

- LLMs: pretrained on large and diverse corpora

Chatbot, translation, text summarization, classification, etc., or as **zero-shot models**

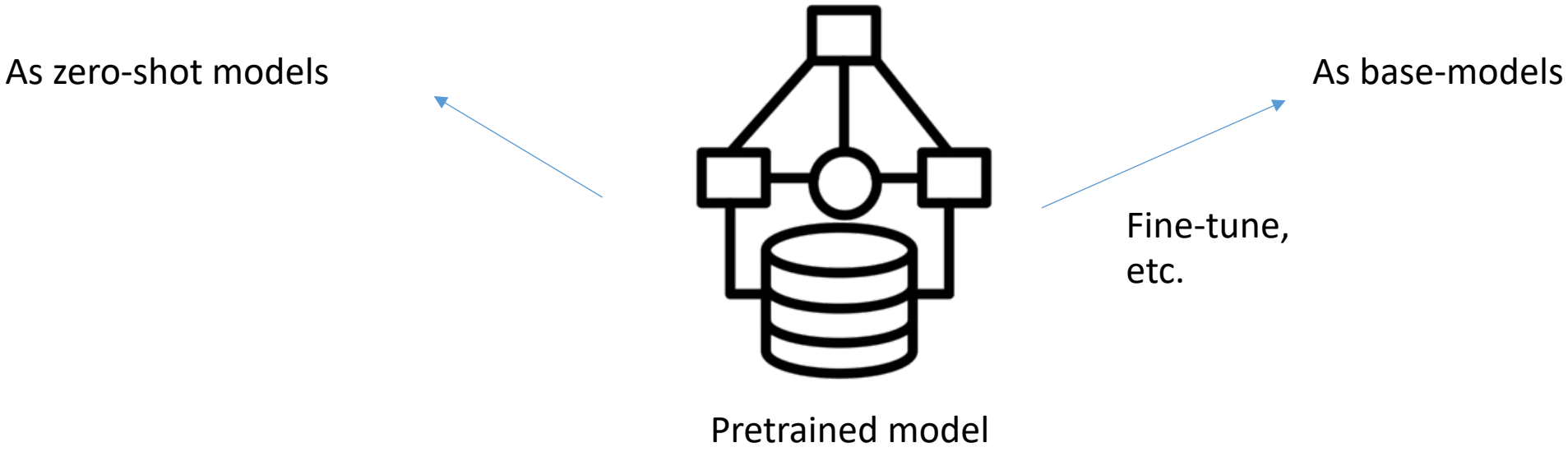
Fine-tune/ RAG, etc.

Legal document analysis, customer support, technical document assistance, etc., or as **base models**

- Benefits:
  - More resource efficient
  - Incredible performance

Can we do the same for ML4DB?

- Pretrained Models: pretrain on diverse databases, configurations, and workloads



- Benefits:
  - More resource efficient
  - Better performance

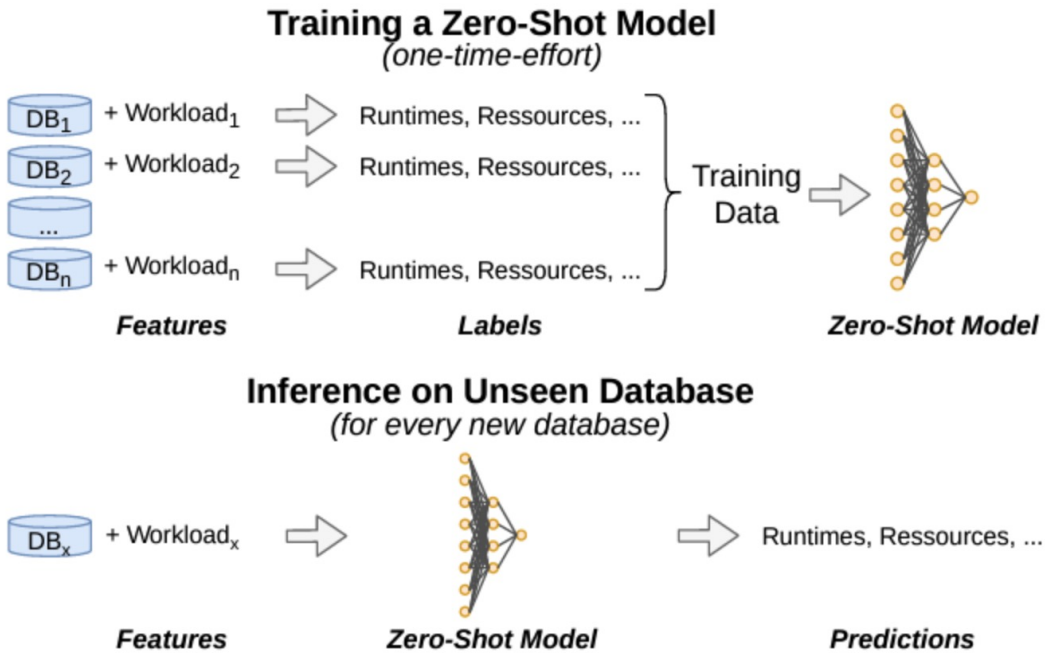
Zero-shot models

- Issues with workload-driven learning
  - Require running **huge** # of queries to get training data
  - Re-run training queries to support new databases, or even when data is updated
- Idea: use a pre-trained model that can generalize to **unseen databases** (with different data characteristics) **out-of-the-box**

Hilprechet & Binnig. One Model to Rule them All: Towards Zero-Shot Learning for Databases. CIDR 22.

Zero-shot models

- A pre-trained model that can generalize to **unseen databases** (with different data characteristics) **out-of-the-box**



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Zero-shot models

- Challenge: ML4DB systems typically encodes features specific to a database, i.e., a table, a column, etc., which are inconsistent for multiple databases

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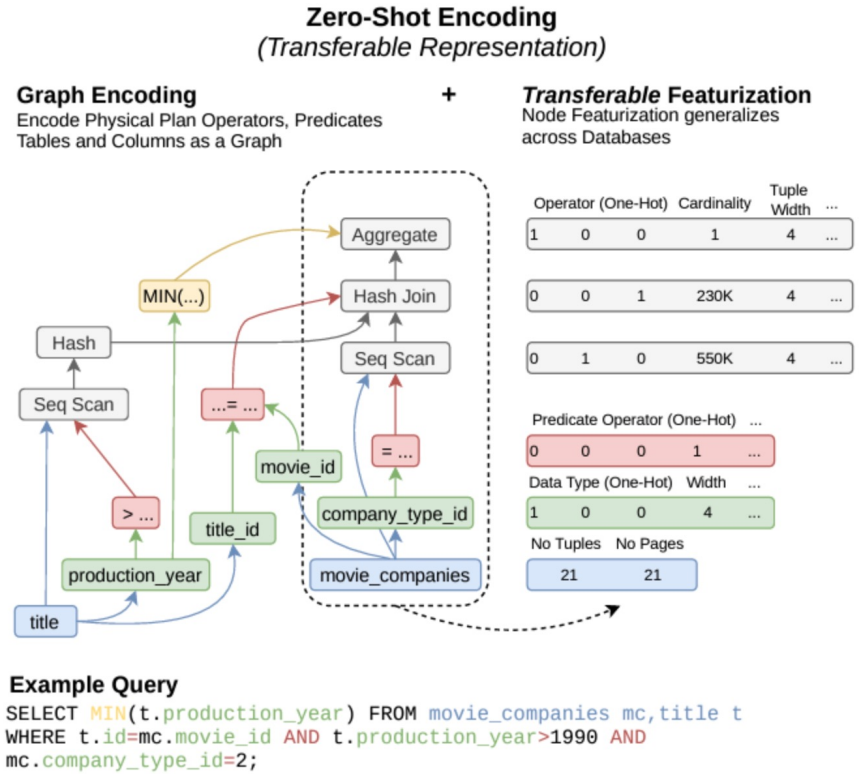
Zero-shot models

- Challenge: ML4DB systems typically encodes features specific to a database, i.e., a table, a column, etc., which are inconsistent for multiple databases
- Solution: Design transferrable (database-agnostic) features

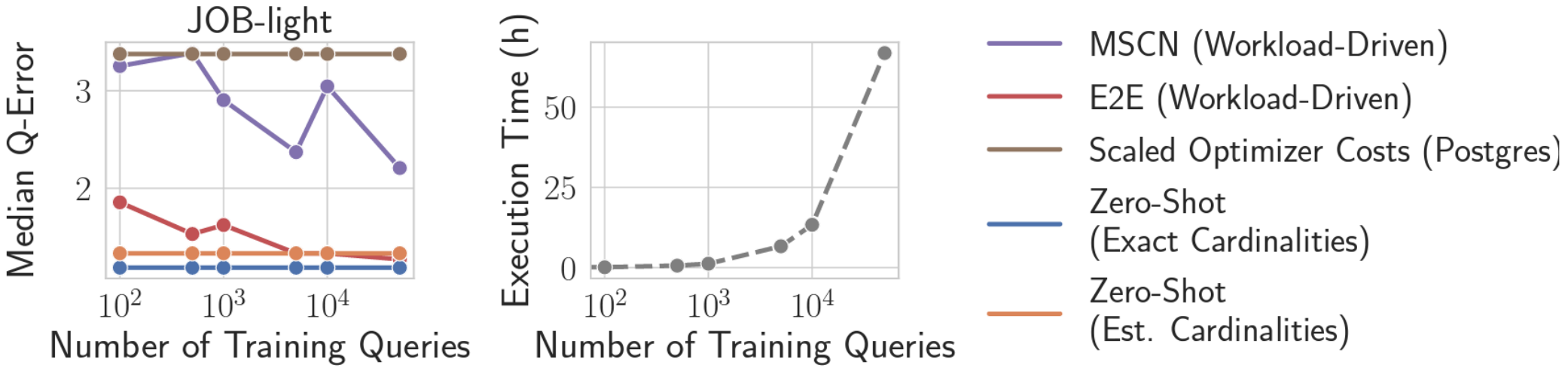


Transferrable Featurization
Data Type,Tuple Width, etc., instead of column name

Benjamin H, Carsten B. One Model to Rule them All: Towards Zero-Shot Learning for Databases. CIDR 22.

Zero-shot cost estimation

- Comparison with workload-driven learning
  - Workload-driven models require large execution time to match zero-shot performance



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Other applications of Zero-shot models

- Physical design tuning
  - MV selection: predict benefit of MV candidates using zero-shot models
- Learned Optimizer
  - Enumerate plans and choose cheapest using zero-shot models
- Data Structure Design
- Device Placement
- …

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MTMLF

- Existing ML4DB systems: one task at a time
  - Ignore relations between tasks
    - Redundant learning
    - Not effective
  - Cold start: not transferrable across tasks

Wu, Z , et al. A Unified Transferable Model for ML Enhanced DBMS. CIDR 22.

MTMLF

- Existing ML4DB systems: one task at a time
  - Ignore relations between tasks
    - Redundant learning
    - Not effective
  - Cold start: not transferrable across tasks

- Question
  - What knowledge can be re-used?
  - How do we re-use them?

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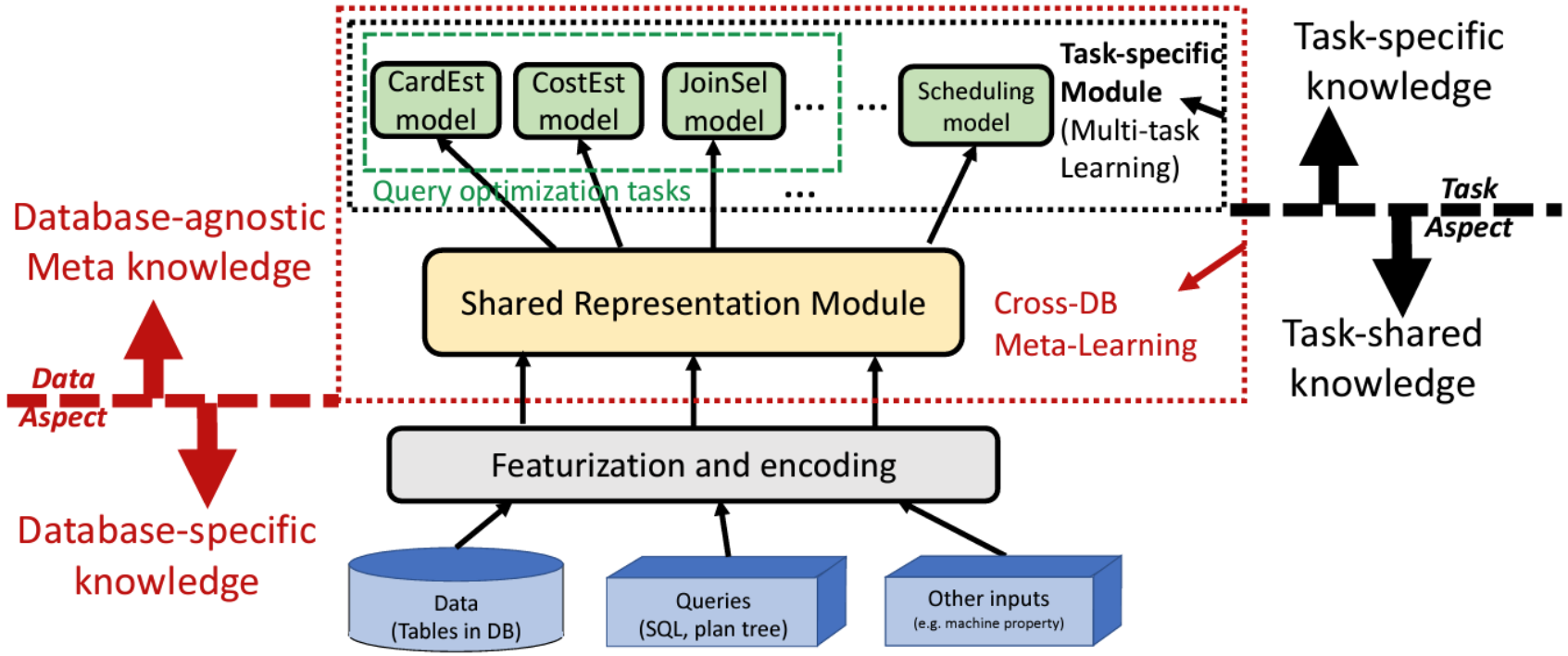
MTMLF

- Learned data and task knowledge decomposition



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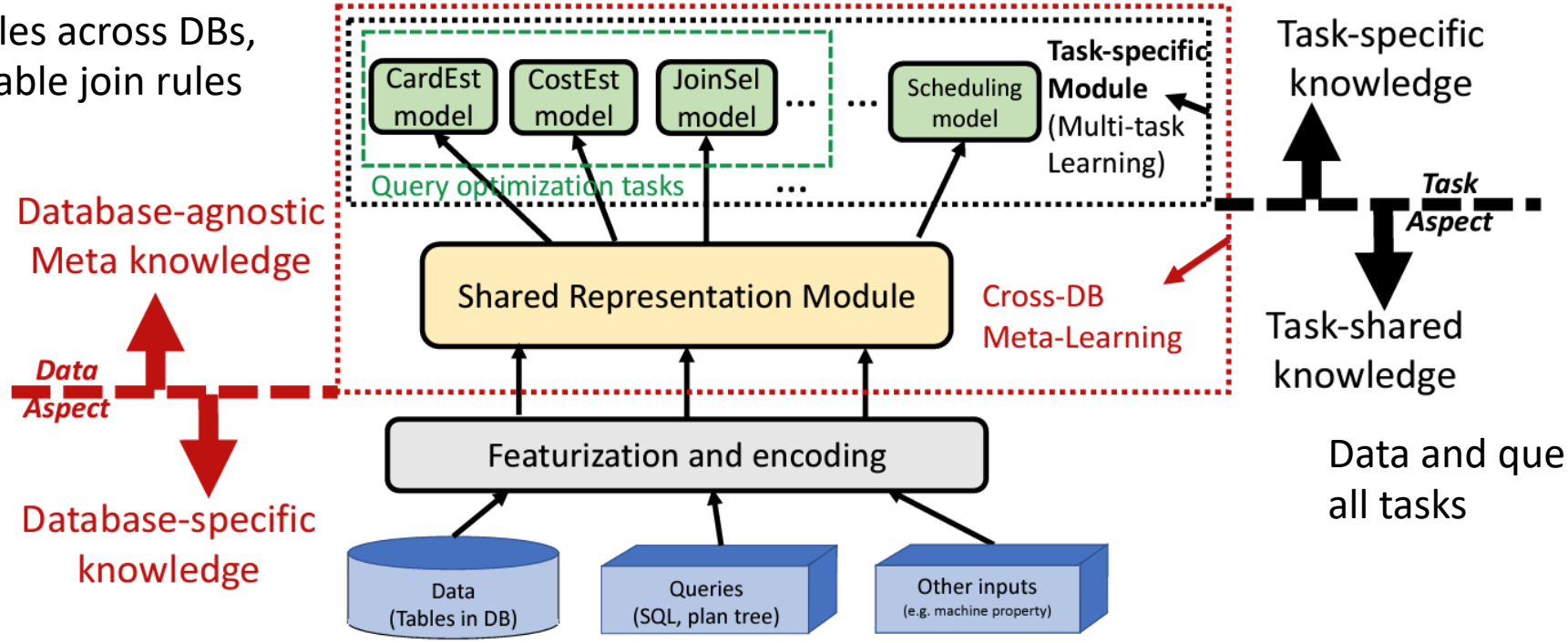
MTMLF

- Learned data and task knowledge decomposition

Method to a specific task, e.g. join order selection rules

Common rules across DBs, e.g., multi-table join rules



Data and query representations in all tasks

Data distributions and join schema

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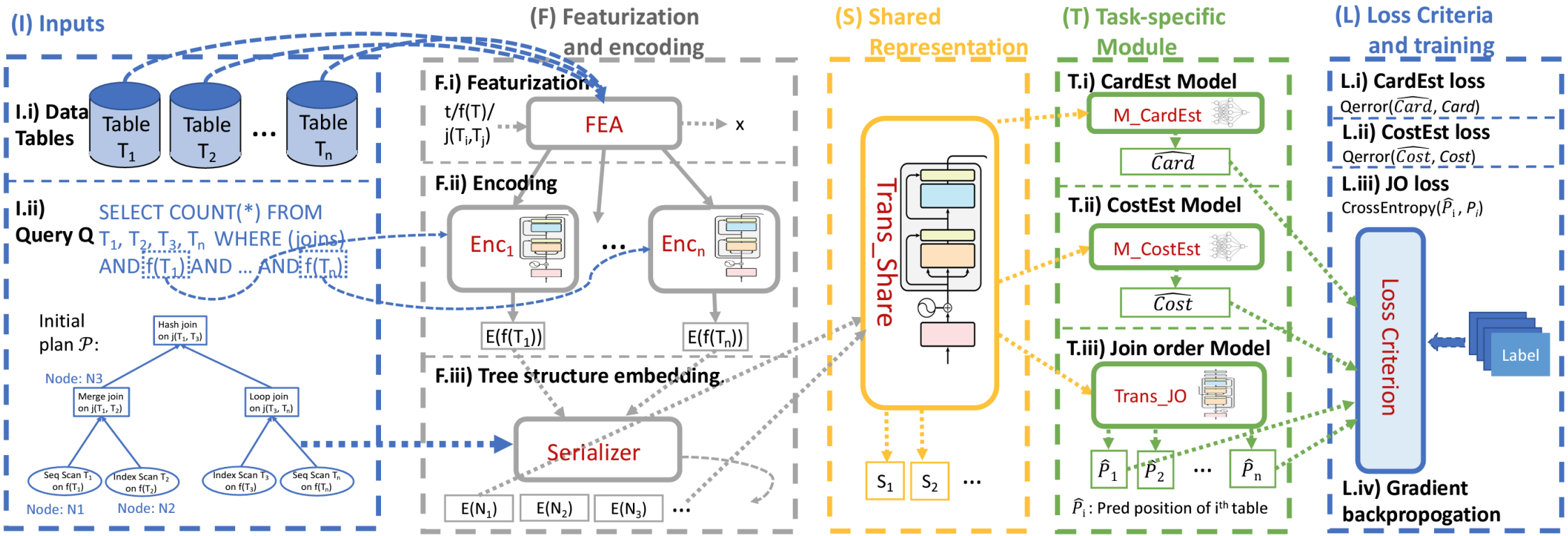
Envisioned DB service

- Service provider:
  - Train on multiple anonymized users DBs
  - Provide users the **shared representation** and **task specific** modules
  - Periodically collect anonymized information and update model as service upgrade
- Users:
  - Train **featurization** module for its own DB
  - Execute a small number of queries to fine-tune model
  - (Optionally) provide anonymized information to service provider

Wu, Z , et al. A Unified Transferable Model for ML Enhanced DBMS. CIDR 22.

Query Optimizer: A Case Study

- Jointly learn 3 tasks



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Case Study Result

- More effective than separate learning

Table 1: Q-errors on the JOB workload.

Method	Cardinality			Cost		
	median	max	mean	median	max	mean
PostgreSQL	184.00	670,000	10,416	4.90	4920	105.00
Tree-LSTM	8.78	696.29	36.83	4.00	290.35	15.01
MTMLF-QO	**4.48**	**614.45**	**28.69**	**2.10**	**37.54**	**4.20**
MTMLF-CardEst	5.12	804.48	36.66	\	\	\
MTMLF-CostEst	\	\	\	2.06	61.41	4.69

Table 2: Execution time with different join orders.

JoinOrder	Total Time	Overall Improvement Ratio
PostgreSQL	1143.2 min	\
Optimal	209.1 min	81.7%
MTMLF-QO	**318.3 min**	**72.2%**
MTMLF-JoinSel	450.4 min	60.6%

Wu, Z , et al. A Unified Transferable Model for ML Enhanced DBMS. CIDR 22.

Case Study Result

- Artificially generated 11 datasets with various distributions and number of tables
- Trained on 10, tested on 1

JoinOrder	Total Time	Overall Improvement Ratio
PostgreSQL	393.9 min	\
MTMLF-QO (MLA)	**234.1 min**	**40.6%**
MTMLF-QO (single)	219.5 min	44.3%

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Pretrained workload characterization

- Workload characterization in databases is important
  - Query plan performance depends on queries, data, and resources
- Challenges:
  - Diverse query structure, high modeling complexity, difficult domain adaptation, etc.

Debjyoti P, et al. Database Workload Characterization with Query Plan Encoders. VLDB 21

Pretrained workload characterization

- Workload characterization in databases is important
  - Query plan performance depends on queries, data, and resources
- Challenges:
  - Diverse query structure, high modeling complexity, difficult domain adaptation, etc.
- Idea:
  - Develop and pre-train a query plan encoder
  - Fine-tune to arbitrary database and task

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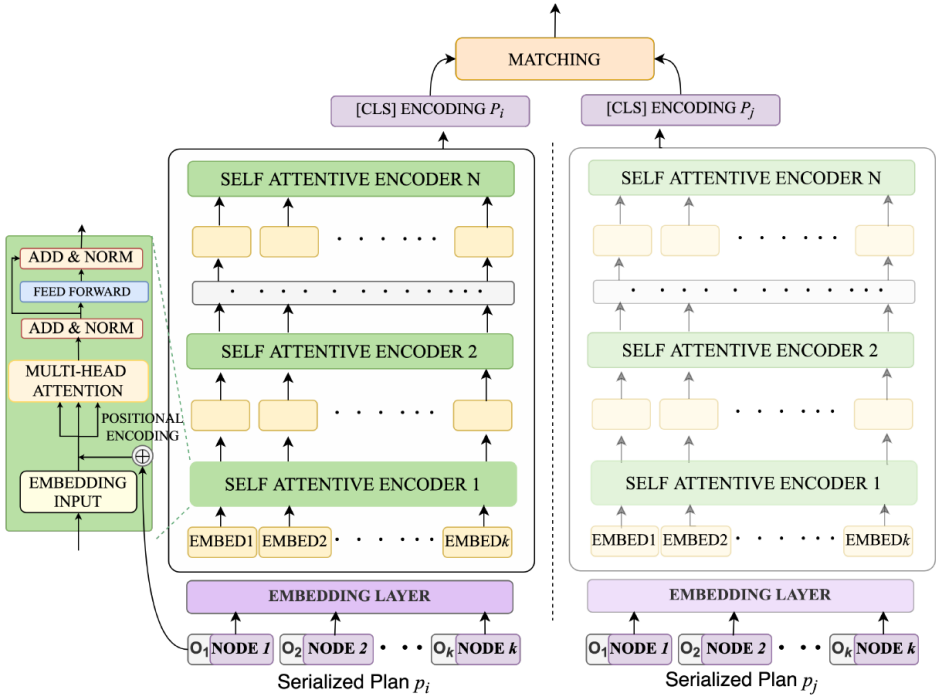
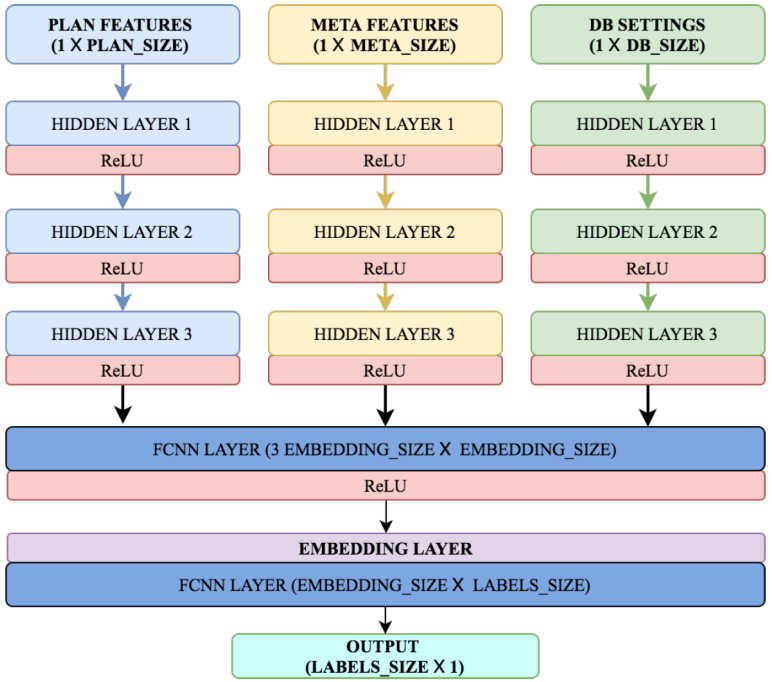
Separate Structural encoder and Performance Encoder

- Separate encoders for structure features and performance features

Train with matching loss



Train with label loss (time, cost, etc)



Structural Encoder

Performance Encoder

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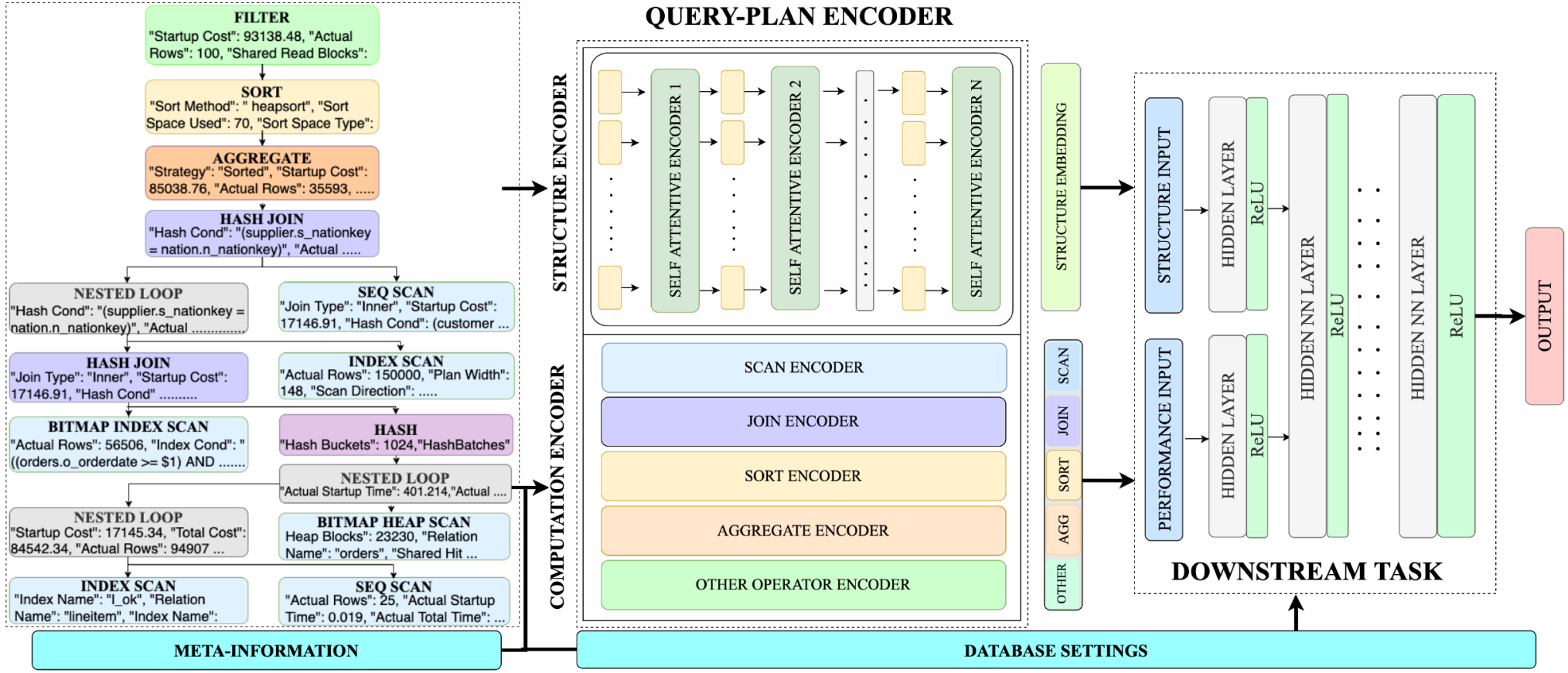
Separate Structural encoder and Performance Encoder

- Full architecture (Both encoder can be used together or separately)



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Experiments

- Pretrain on various sources
  - Structure encoder: crowdsourced plan dataset
  - Performance encoder: TPC-H, TPC-DS
- Fine-tune to downstream tasks

Latency Prediction

Model	$R \leq 1.5$	$1.5 < R \leq 2.0$	$R > 2.0$
TAM	51%	22%	27%
SVM	68%	15%	17%
RBF	85%	6%	9%
QPPNet	89%	**7%**	4%
Plan Encoder	**91%**	**7%**	**2%**

Query Classification

Models	Development		Test	
	template	cluster	template	cluster
Structure only	0.2452	0.4670	0.1946	0.3847
Performance only	0.1645	0.2973	0.0977	0.1769
Both encoders	**0.2783**	**0.5573**	**0.2518**	**0.4647**
Both encoders 10% data	0.2000	0.4927	0.151	0.334
Both encoders 30% data	0.2555	0.5228	0.1843	0.3855

Debjyoti P, et al. Database Workload Characterization with Query Plan Encoders. VLDB 21

Take-aways for Pre-trained Models

- We can exploit pre-training techniques to reduce redundant computations by
  - Disentangle model components
  - Design more robust featurization methods
  - Employ multi-task learning techniques

- Early-stage idea
  - Proof-of-concept
  - How to collect pretraining dataset?

Tutorial Overview

- ML4DB Foundations
- ML4DB Paradigms
- ML4DB Open problems

ML4DB Paradigms

- “Replacement” Paradigm
  - Machine learning models replace the traditional database components
  - Example: replacing index, replacing query optimizer

- “ML-enhanced” Paradigm
  - Machine learning models improve the traditional database components
  - Example: learn better policies during index organization, generate helpful hints for expert optimizer

“Replacement” Paradigm

- Learned index: Replace the **B-tree Index** with a **cumulative density function (CDF)** model

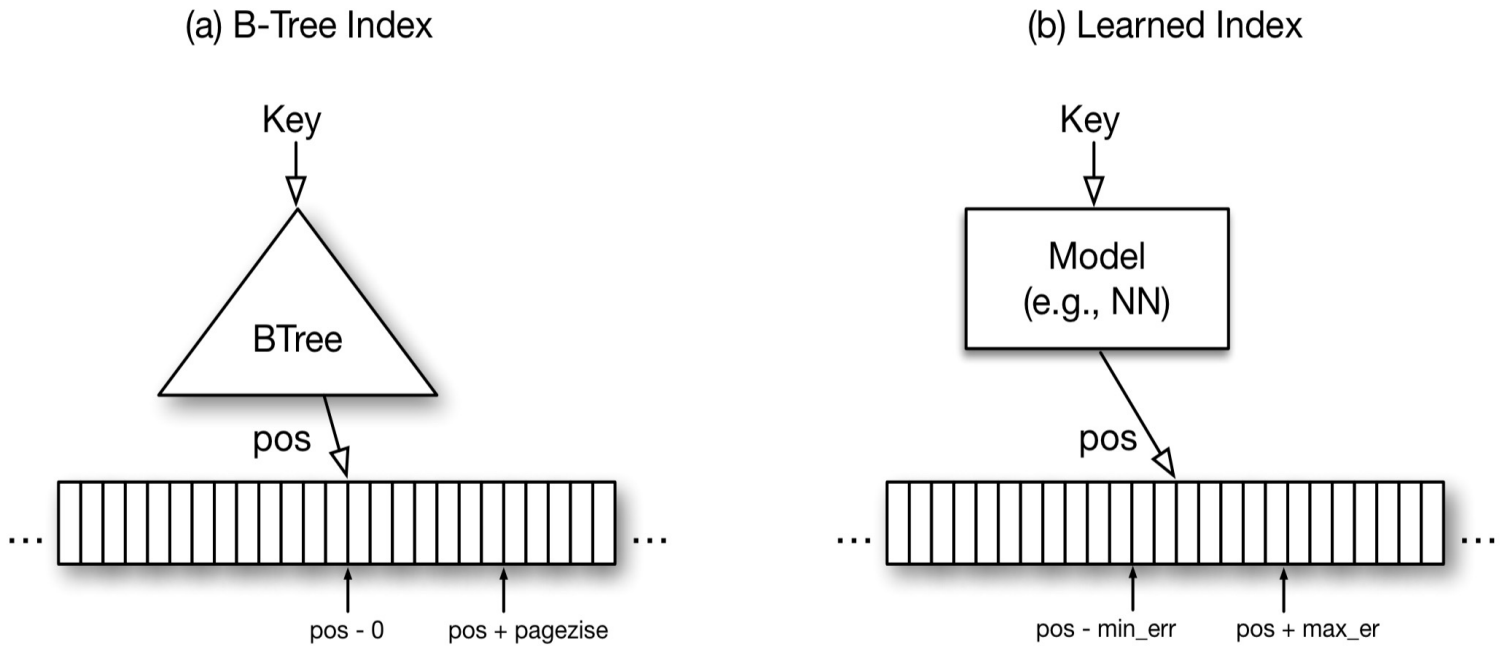


Figure from Tim Kraska et al. **The case for learned index structures.** SIGMOD’18

“ML-enhanced” Paradigm

- ML-enhanced index: Use machine learning to **improve** operations in **traditional R-tree index**, e.g., data insertion

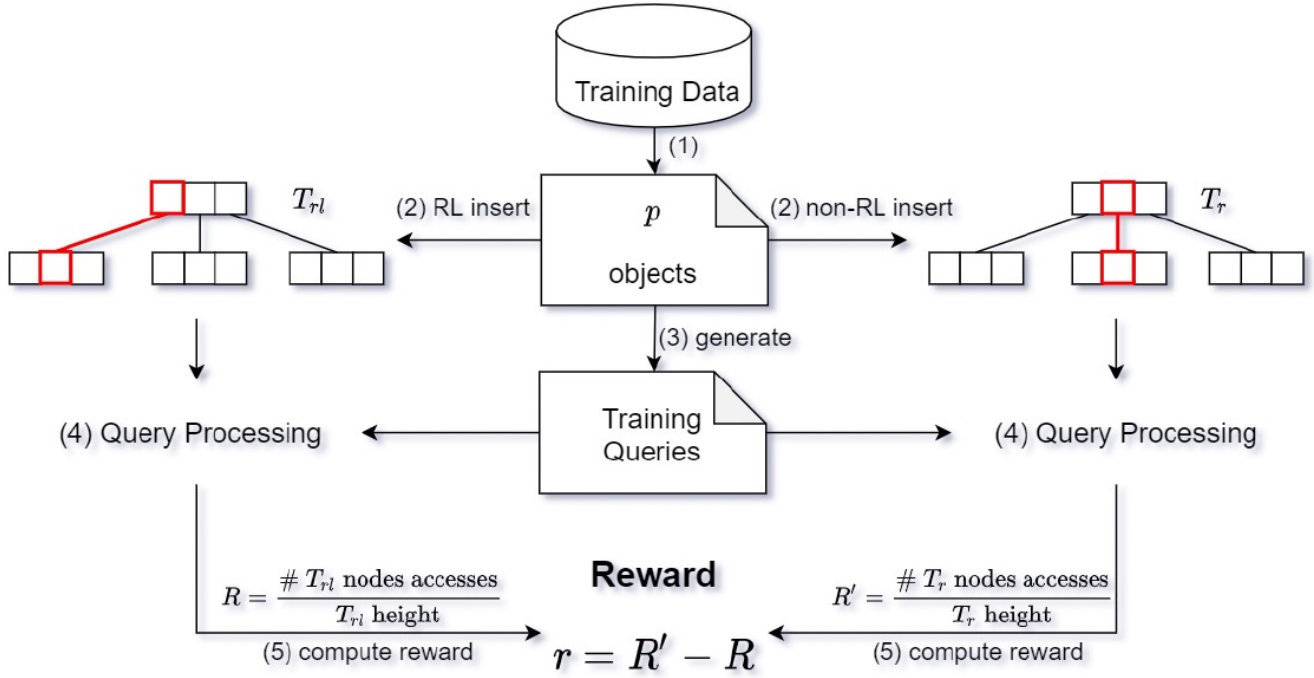


Figure from Tu Gu et al. **The RLR-Tree: A Reinforcement Learning Based R-Tree for Spatial Data.** SIGMOD’23

“Replacement” Paradigm

- Learned query optimizer: Replace **optimizer** with a **reinforcement learning** model

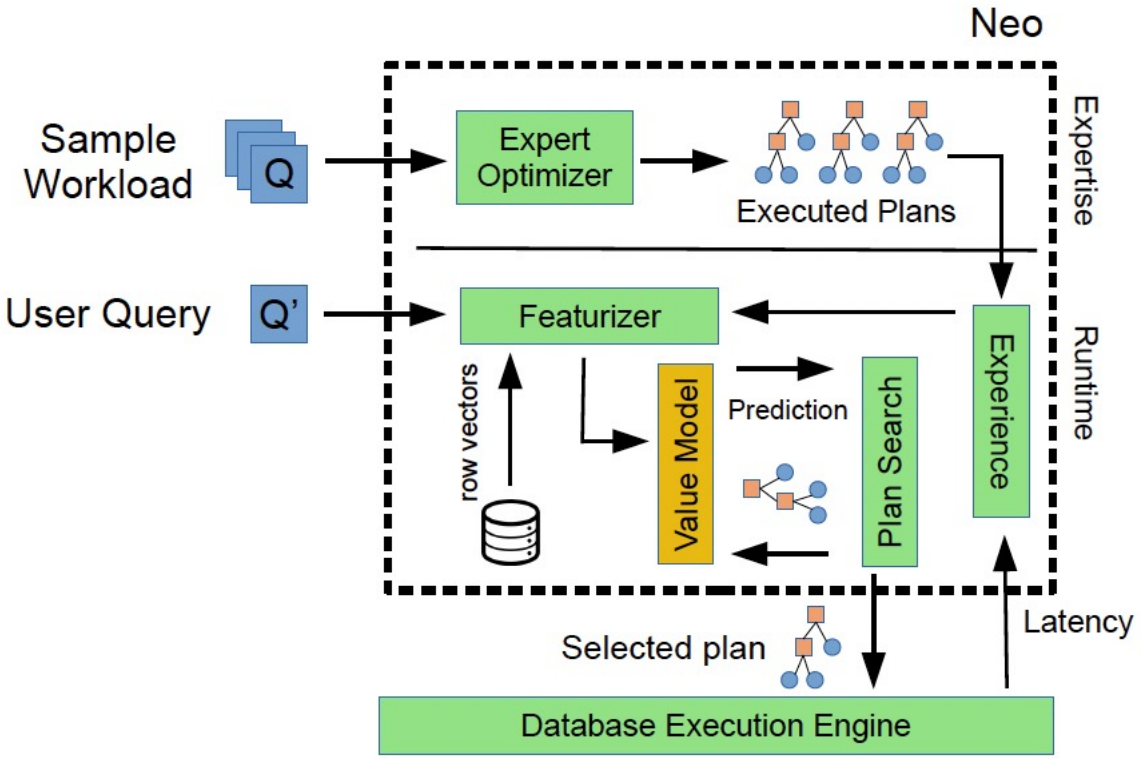


Figure from Ryan Marcus et al. **NEO: a learned query optimizer.** SIGMOD’19

ML4DB Paradigms

- ML-enhanced query optimizer: Use machine learning to **improve expert query optimizer**, e.g., provide a set of hints

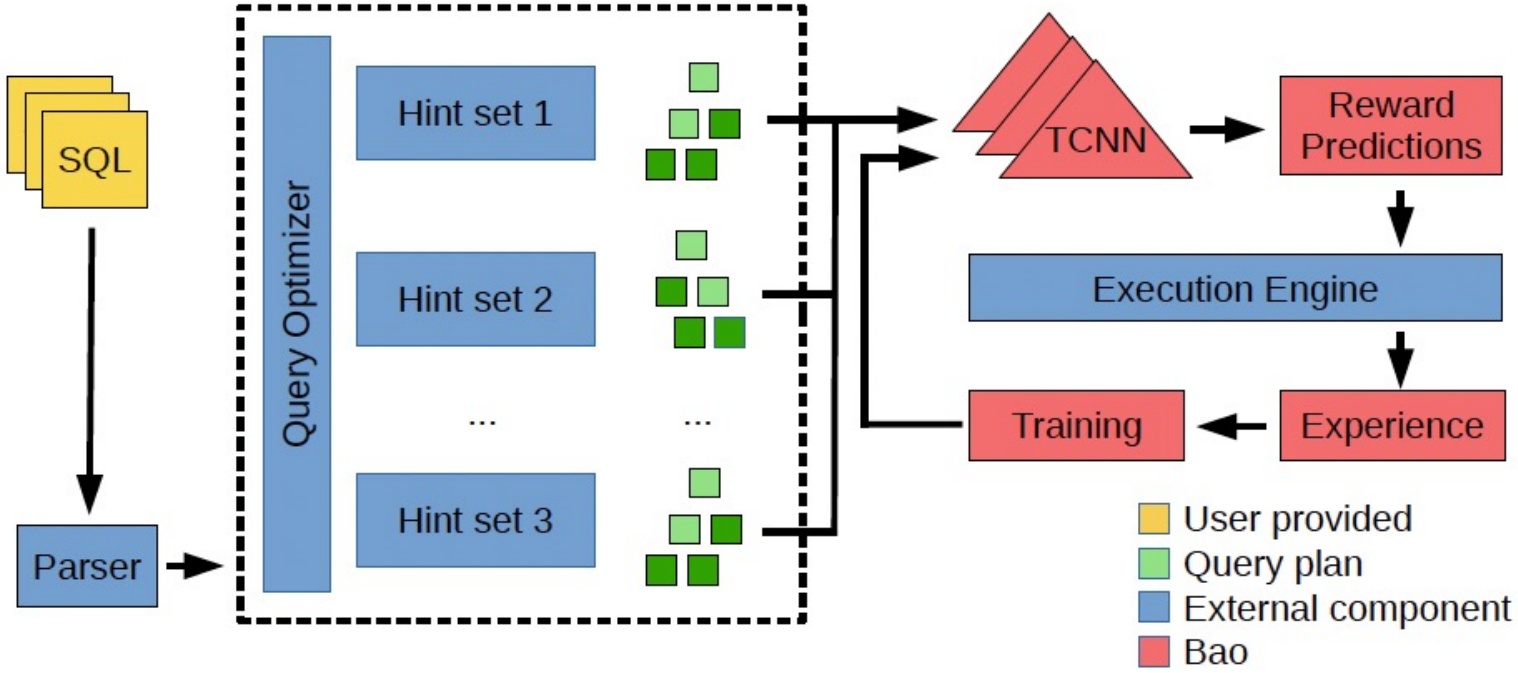
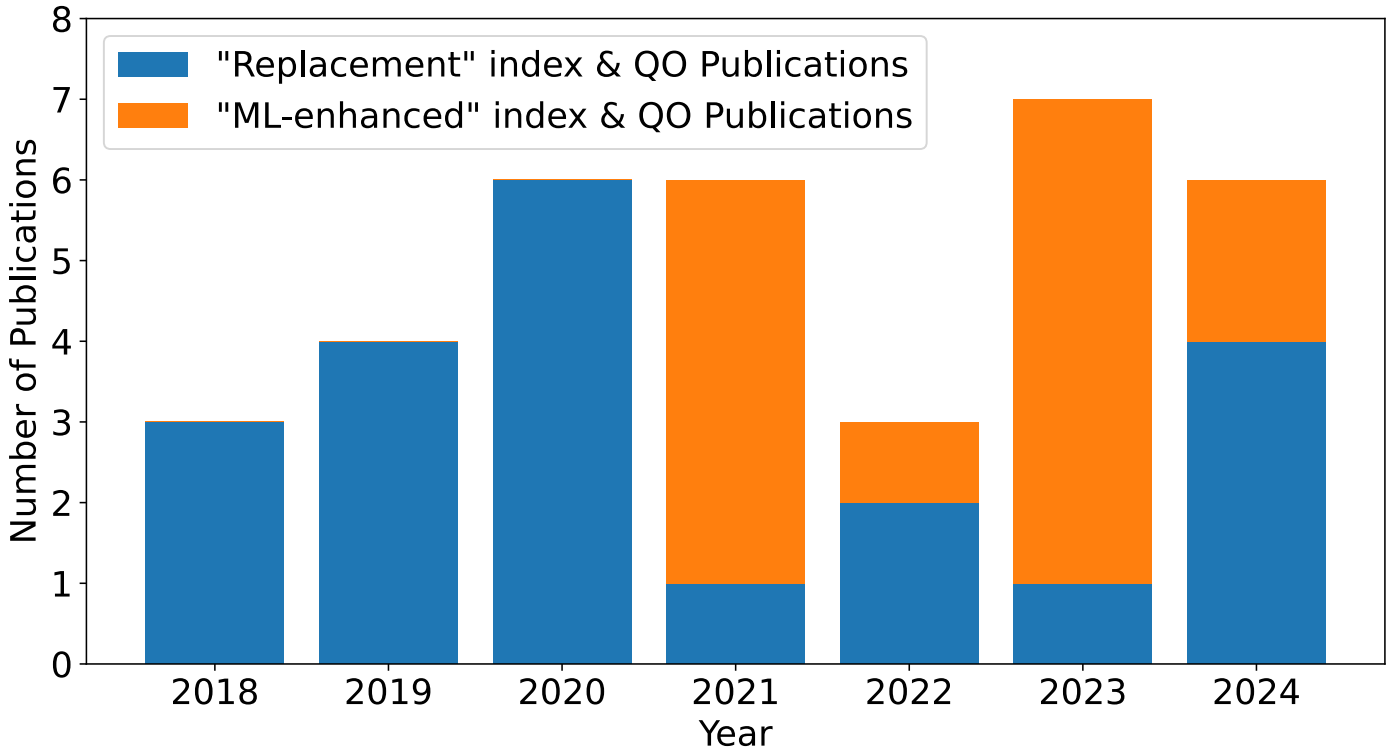


Figure from Ryan Marcus et al. **BAO: Making learned query optimization practical.** SIGMOD'21

Publication Trend

- We observe a noticeable shift from the “Replacement” paradigm to the “ML-enhanced” paradigm over the past years.



Publication on machine learning for index & Query Optimizer (QO) in SIGMOD and VLDB

ML4DB Paradigms

- We study ML4DB paradigms from the perspective of two important problems
  - Database indexing
  - Query optimization

ML4DB Paradigms

- We study ML4DB paradigms from the perspective of two important problem
  - Database indexing
  - Query optimization

ML4DB Paradigms in Database indexing

- Part 1: Preliminary
- Part 2: Learned index
- Part 3: ML-enhanced index
- Part 4: Summary

B+-tree Index

- B+-tree builds a balanced tree over the keys, which enables $O(\log n)$ key lookup.
- Support fast insertion and deletion of data - $O(\log n)$.

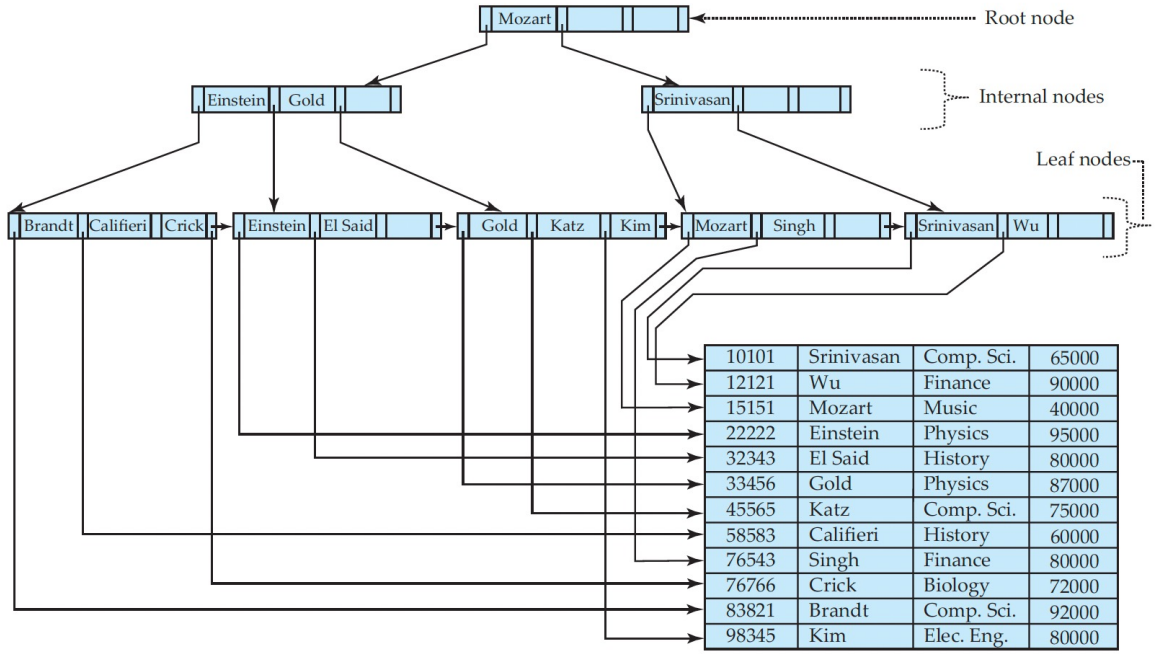
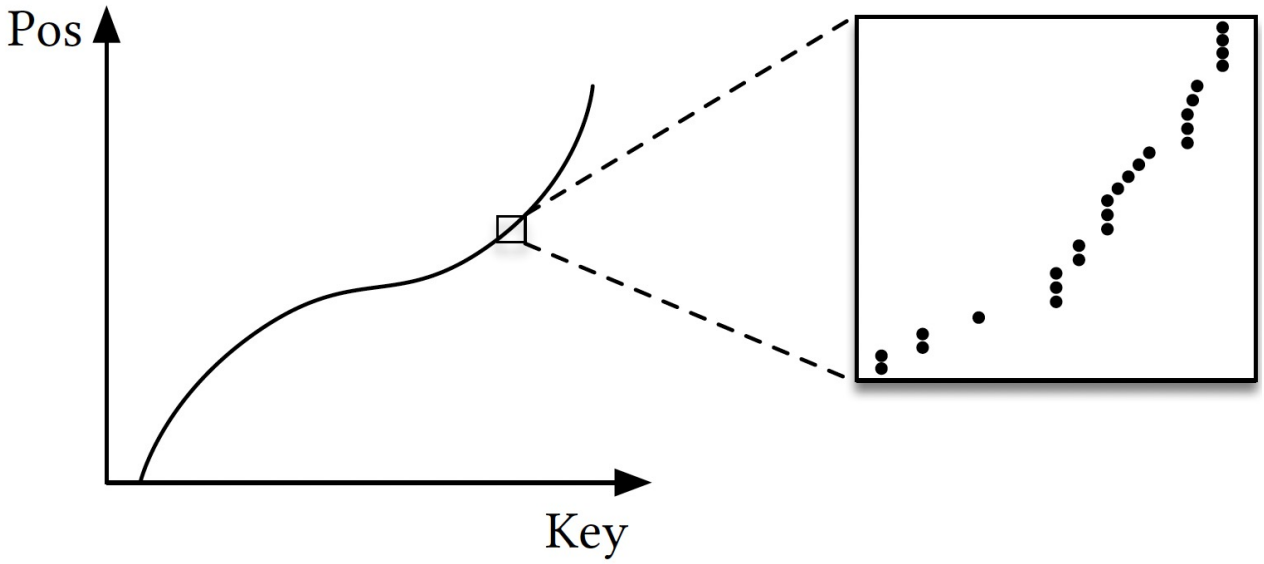


Figure from **Database System Concepts, 6th Edition.**

Learned index

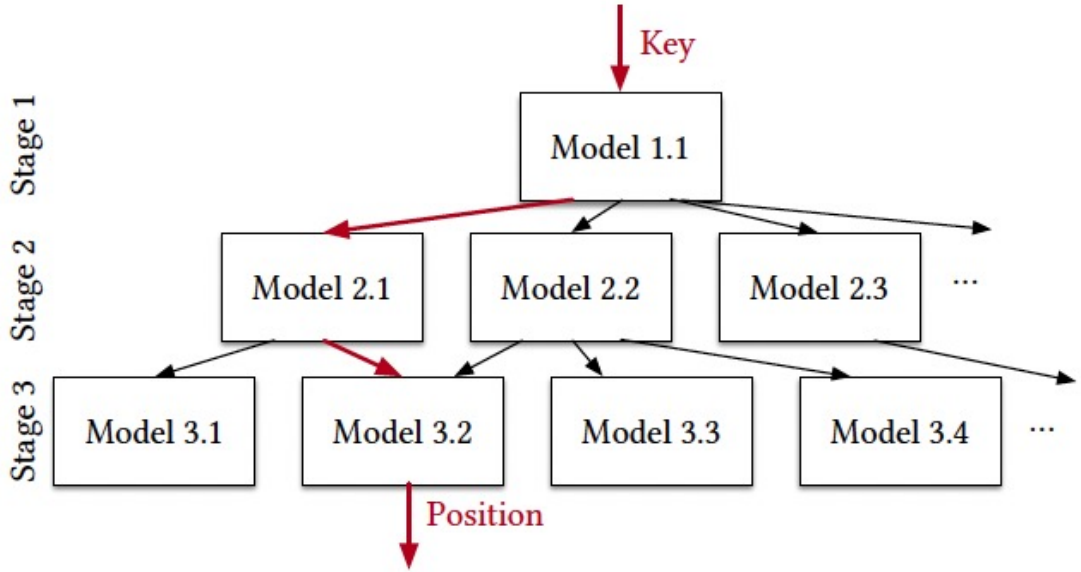
- Observation: B+-tree can be considered as a model.
  - Input: Search key
  - Output: Position of the record in a sorted file, i.e., page id
- B+-tree can therefore be replaced by a Cumulative Density Function (CDF) model
  - $p = F(key) * N$



Tim Kraska et al. **The Case for Learned Index Structures.** SIGMOD'18

Learned Index

- The Recursive Model Index (RMI) consists of a hierarchy of models.
- At each stage the model takes the key as an input and picks another model based on output.
- The final stage models predict the position.



Tim Kraska et al. **The Case for Learned Index Structures.** SIGMOD'18

Learned Index

- Improving lookup performance: $O(\log n) \rightarrow O(1)$
- Offload computation from the CPUs to GPUs.
- Space saving: Disk page -> Memory

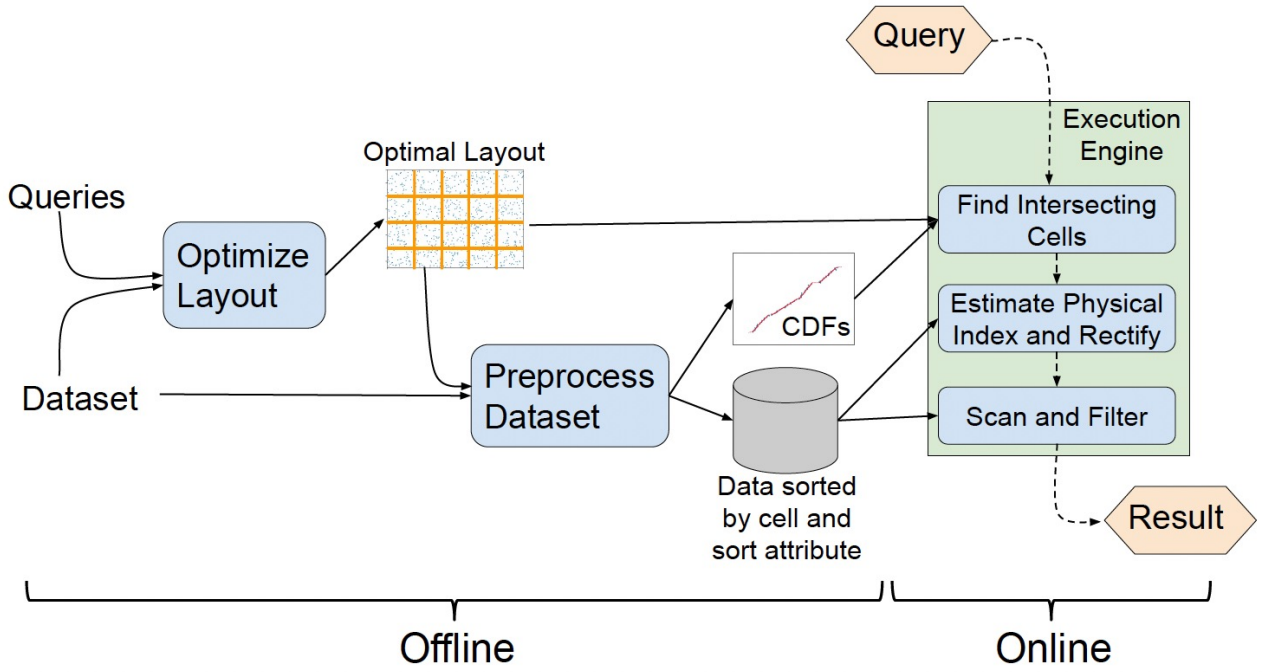
Tim Kraska et al. **The Case for Learned Index Structures.** SIGMOD'18

Learned Index

- A long line of work follows the RMI and improves it in various aspects
- Handling updates
  - Ding et al. ALEX: an updatable adaptive learned index. SIGMOD'20
- Provable bounds
  - Ferragina et al. The PGM-index: a fully-dynamic compressed learned index with provable worst-case bounds. VLDB'20
- Different storage medium
  - Lu et al. APEX: A High-Performance Learned Index on Persistent Memory. VLDB'21
- ……

Learned Multi-dimensional index

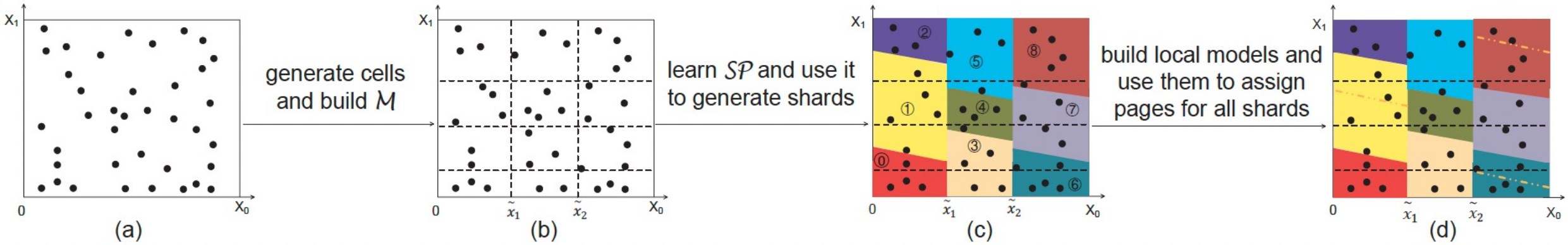
- Flood customizes the data layout to optimize query performance.
- Using empirical CDF models to flatten data into a more uniform space.



Vikram Nathan et al. **Learning Multi-dimensional Indexes.** SIGMOD'20

Learned Spatial Index

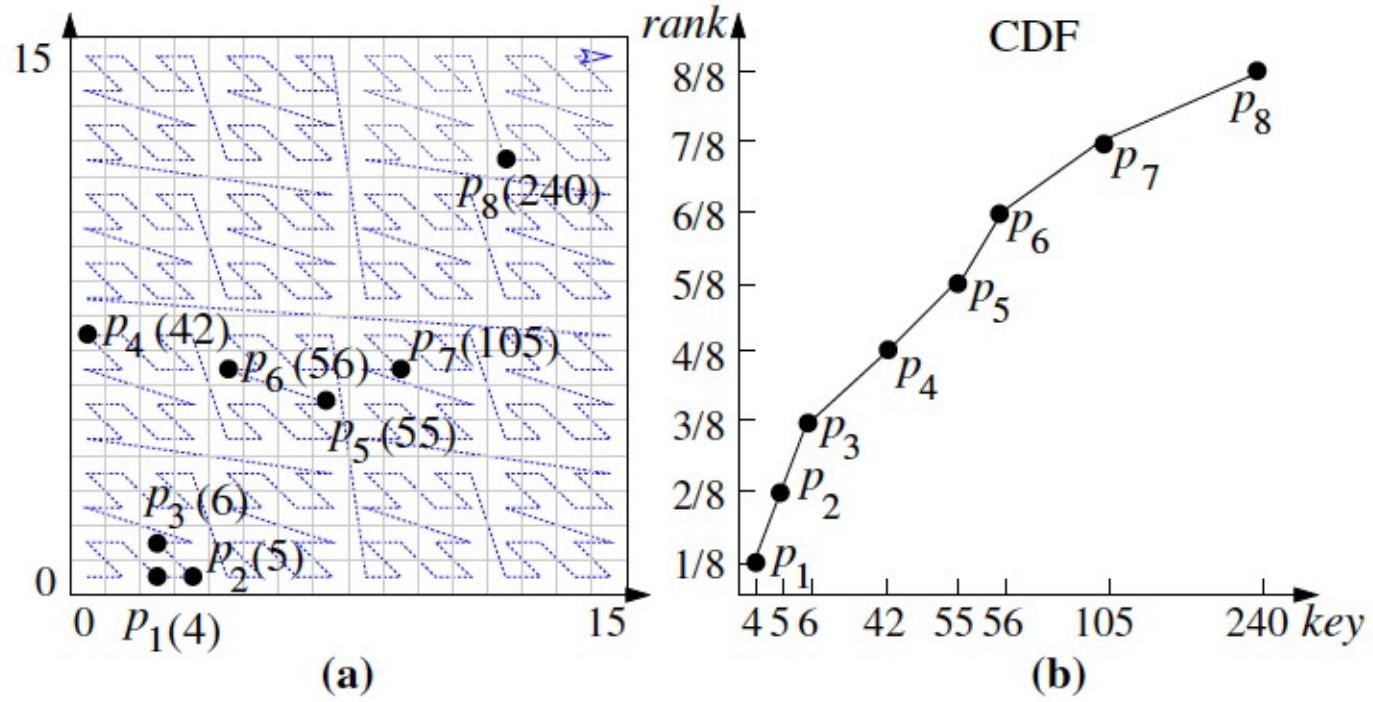
- Learned spatial indexes learns to map spatial coordinate → storage id.
- Specialized Models: a hierarchical structure
  - Grid cells
  - Shard Prediction Functions
  - Local models



Pengfei Li et al. **LISA: A learned index structure for spatial data.** SIGMOD'20

Learned Spatial Index

- Utilize a space-filling curve to linearize spatial coordinates into 1d value.
- Learn a CDF of the linearized values using a learned 1D index.



Jianzhong Qi et al. **Effectively learning spatial indices.** VLDB'20

Motivation for ML-enhanced Index

- **Robustness**:
  - Replace both the index structures and query processing algorithms currently used by the database systems **-->** hard to deploy in existing systems
- **Traditional index has better generalization capability**:
  - Support for more types of data
  - Support for more types of queries
  - Update and deletion handling

- Can we improve the traditional index without replacing the index structure or the query processing algorithm?

ML-enhanced Index

- We will discuss ML-enhanced methods that aid three types of index operations.
- **Insertion**: Building a better index for dynamic data.
  - RLR-tree: learning to improve R-tree insertion
  - BM-tree: learning to design space filling curve
- **Bulk-loading**: Constructing a better index through bulk-loading.
  - PLATON: R-tree packing with learned partition policy
- **Query**: Optimizing index search operation.
  - AI+R-tree: learning to accelerate R-tree search

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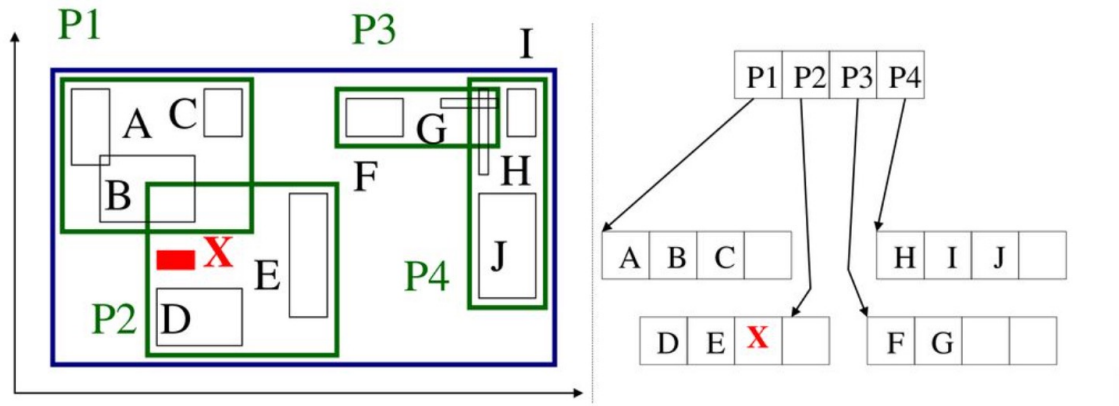
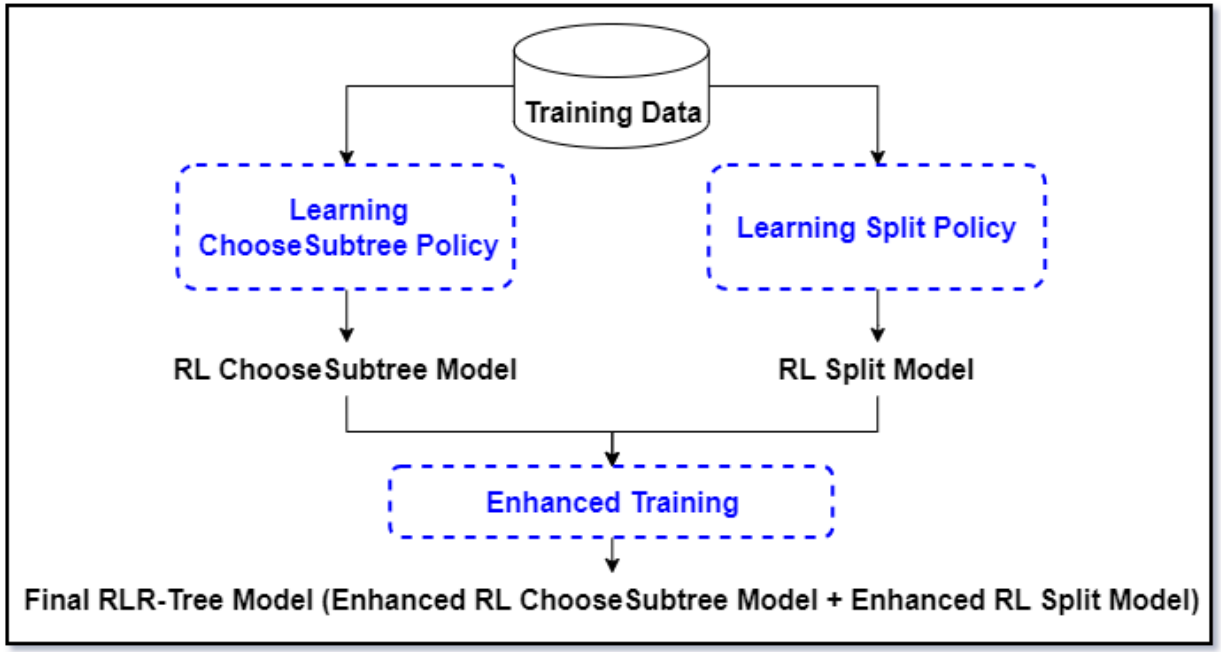
R-tree Insertion

- Two key operations of R-Tree, i.e., **ChooseSubtree** and **Split**.
  - **ChooseSubtree**: starting from the tree root, recursively choose which child node to insert the new data object, until a leaf node is reached.
  - **Split**: If the number of entries in a node exceeds the capacity, the Split operation is invoked to divide the entries into two groups.
- **Variants of R-tree have different hand-crafted heuristics. But no single heuristic rule is dominant**.



RLR-Tree Overview

- **RLR-Tree:** use **machine learning (ML) to construct a better R-Tree** for better query efficiency in a dynamic environment.
  - Model ChooseSubtree and Split as two Markov Decision Processes (MDPs) and train **reinforcement learning (RL) models** to learn optimal policies.



Tu Gu et al. **The RLR-Tree: A Reinforcement Learning Based R-Tree for Spatial Data.** SIGMOD'23

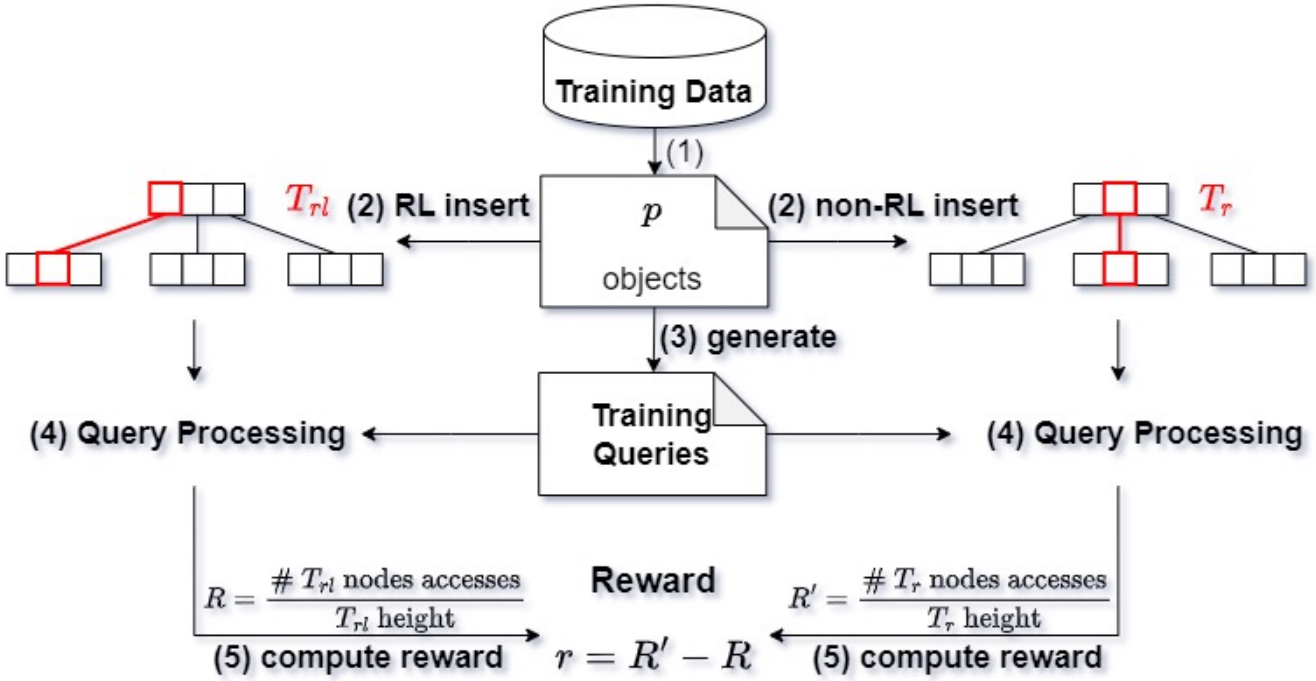
RLR-Tree ChooseSubtree

- Key Features of RL ChooseSubtree:
  - **Action Space**:
    - Setting existing hand-crafted heuristic strategies as actions is straightforward, but experimentally shown not to work.
    - Select the top k child nodes to form the action space. With "bad" actions removed, model training gets more efficient.
  - **State Space**:
    - Using the extreme values of the minimum bounding box of each node (action) as state features is straightforward, but experimentally shown not to work.
    - Instead, capture the change resulted from each action, such as increase in the area and the perimeter of the candidate child node.

Tu Gu et al. **The RLR-Tree: A Reinforcement Learning Based R-Tree for Spatial Data.** SIGMOD'23

RLR-Tree ChooseSubtree

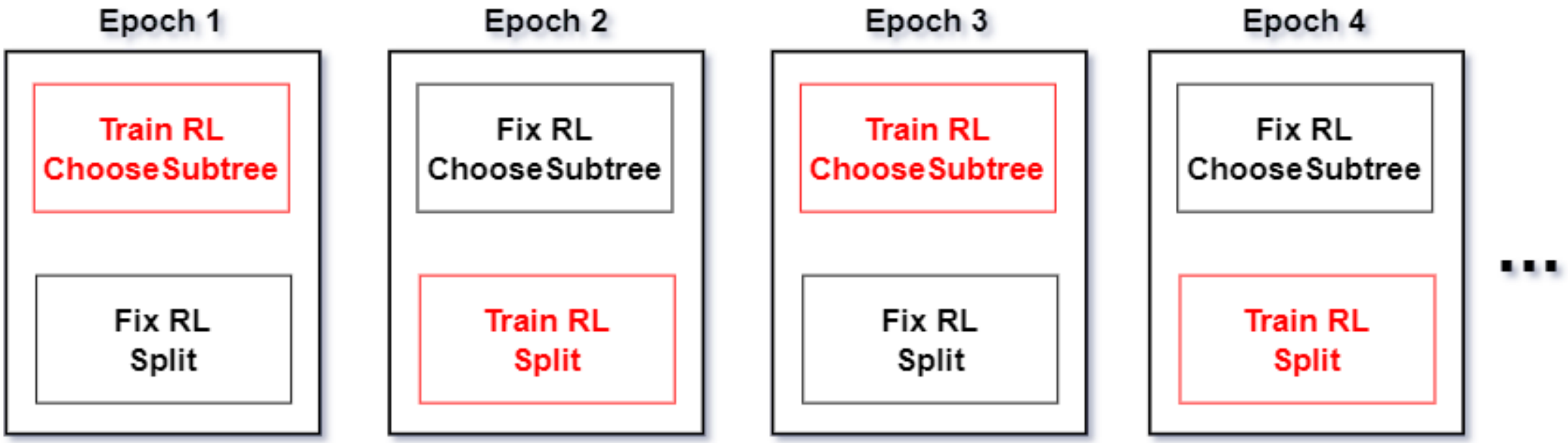
- Key Features of RL ChooseSubtree:
  - **Reward Computation:** construct an RLR-Tree (T_{rl}) and an R-Tree (T_r) and measure the difference in their query performance.



Tu Gu et al. **The RLR-Tree: A Reinforcement Learning Based R-Tree for Spatial Data.** SIGMOD'23

RLR-Tree Enhanced Training

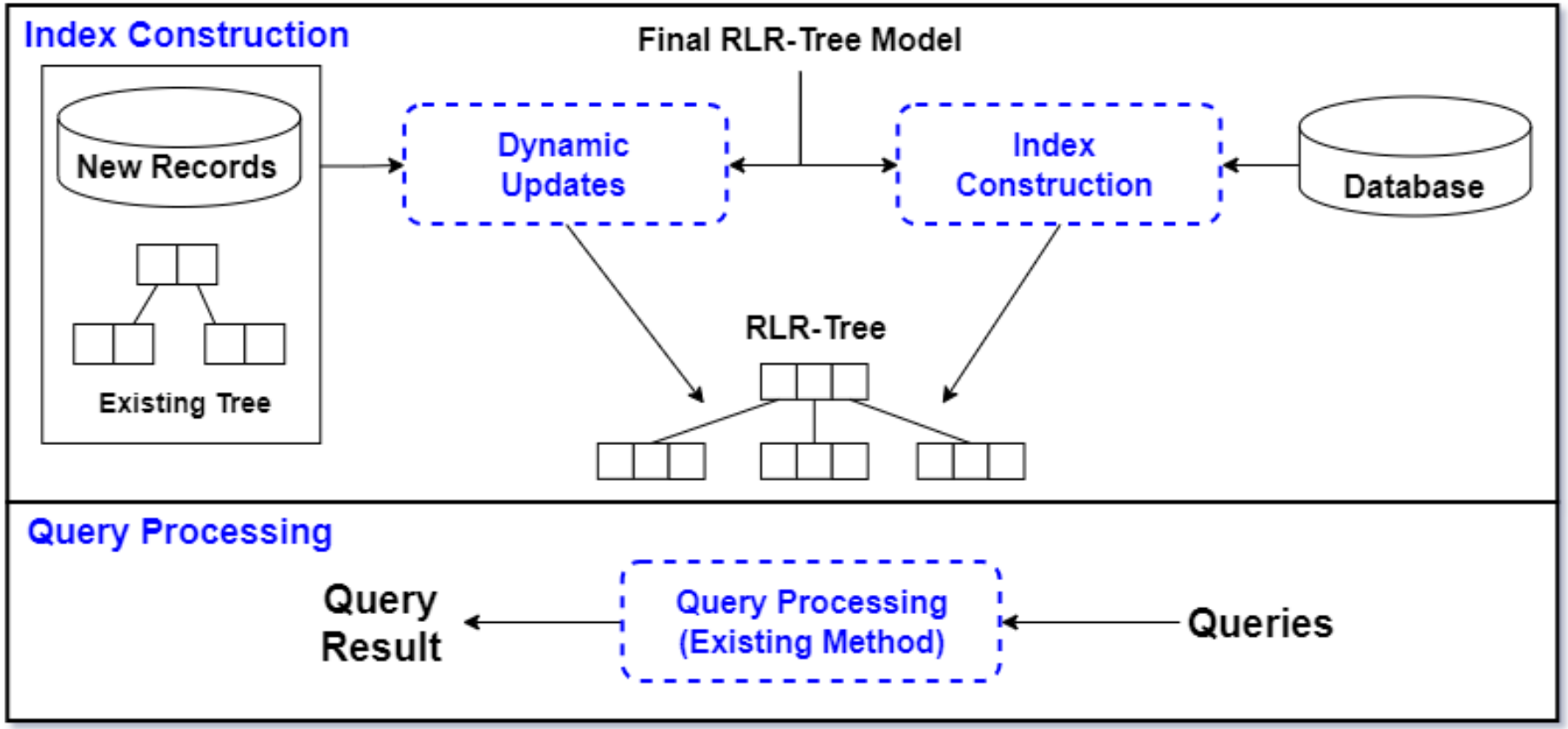
Train the RL agents for ChooseSubtree and Split together to further improve their performances.



Tu Gu et al. **The RLR-Tree: A Reinforcement Learning Based R-Tree for Spatial Data.** SIGMOD'23

RLR-Tree Overview

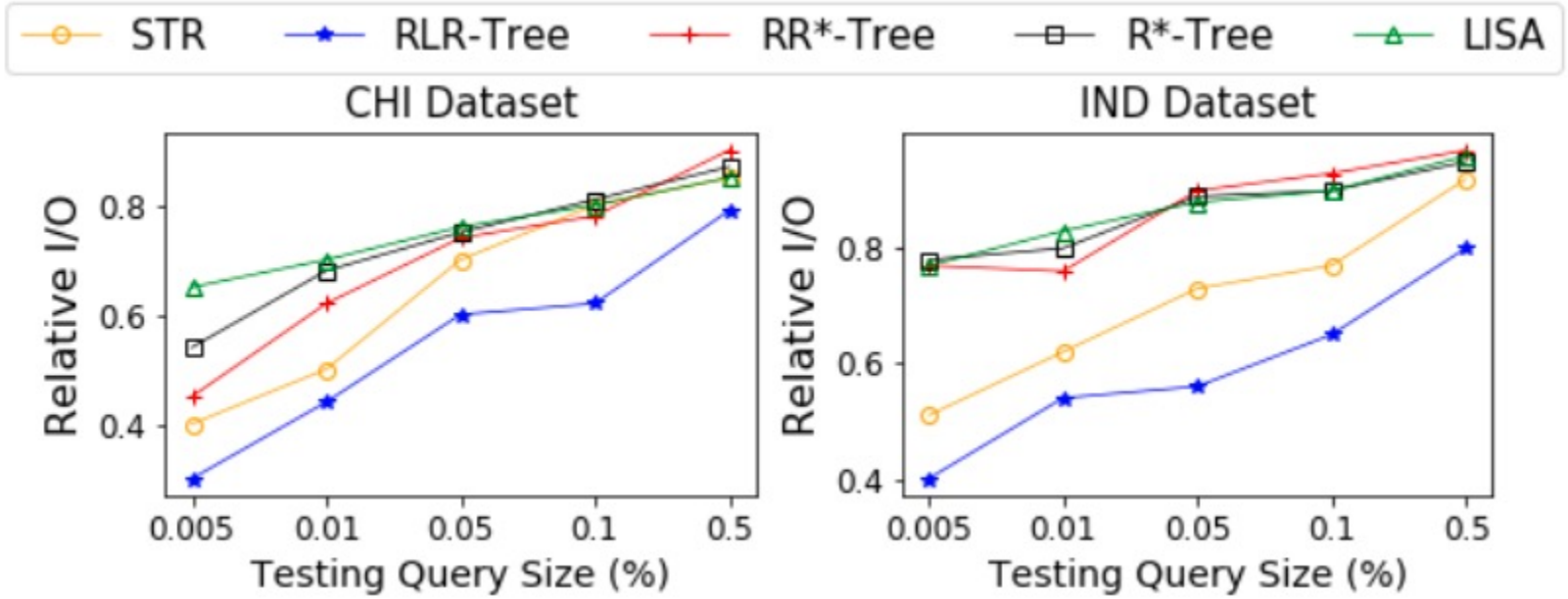
Overview (Index Construction & Query Processing):



Tu Gu et al. **The RLR-Tree: A Reinforcement Learning Based R-Tree for Spatial Data.** SIGMOD'23

Experimental Results

RLR-Tree outperform various R-tree variants on spatial queries.



Tu Gu et al. **The RLR-Tree: A Reinforcement Learning Based R-Tree for Spatial Data.** SIGMOD'23

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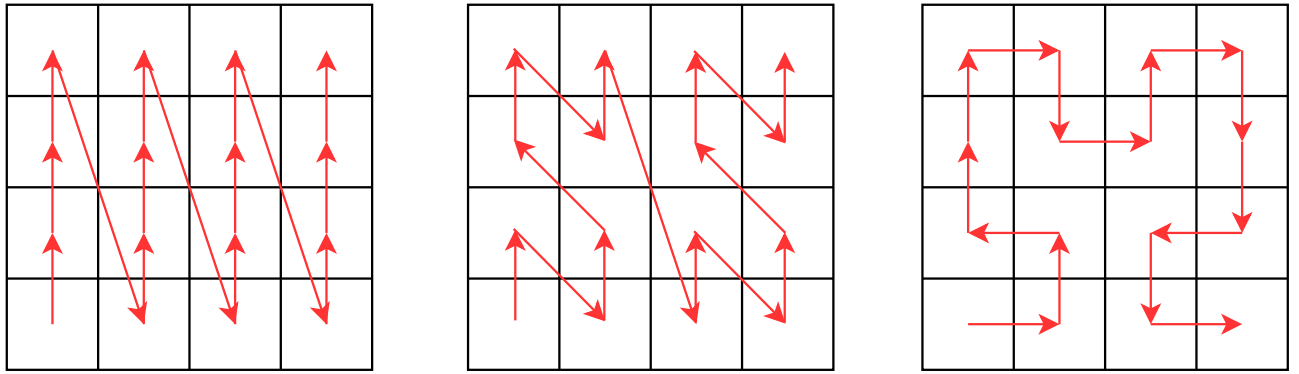
Space-Filling Curve (SFC)

- A SFC is used to map a multi-dimensional data point to a 1d value
- Then a one-dimensional index can be used to index the mapped values
  - B+-tree index
  - Learned indexes



(a) C-curve (b) Z-curve (c) Hilbert curve

- Each type of SFC has a fixed mapping function
- May not fit with different datasets/queries.

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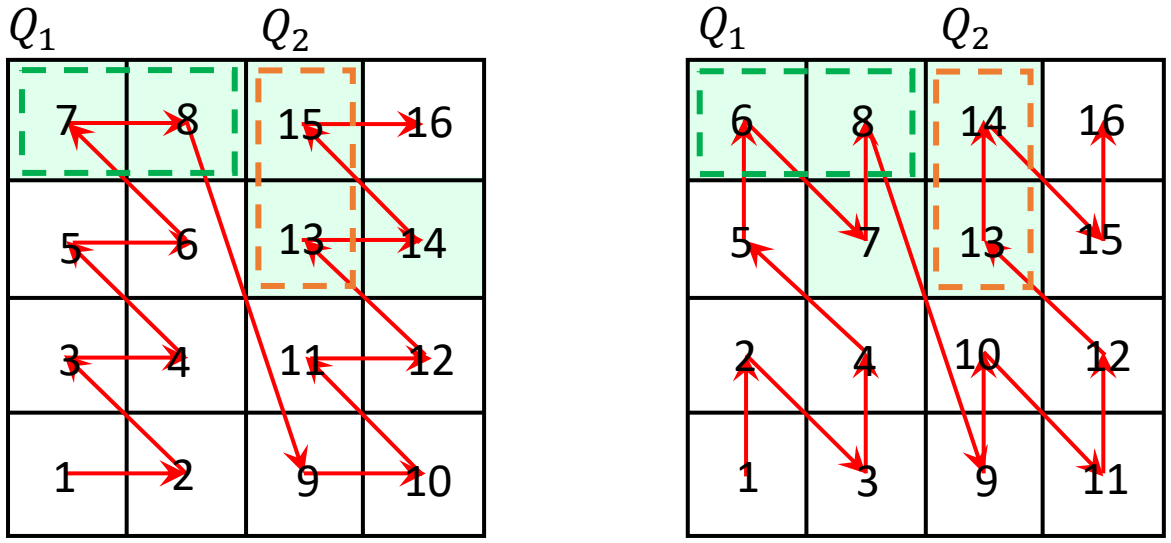
Design instance-optimized SFCs

- No single SFC can dominate the performance on all datasets and query workloads



(a) SFC-1 works best for Q_1.

(b) SFC-2 works best for Q_2.

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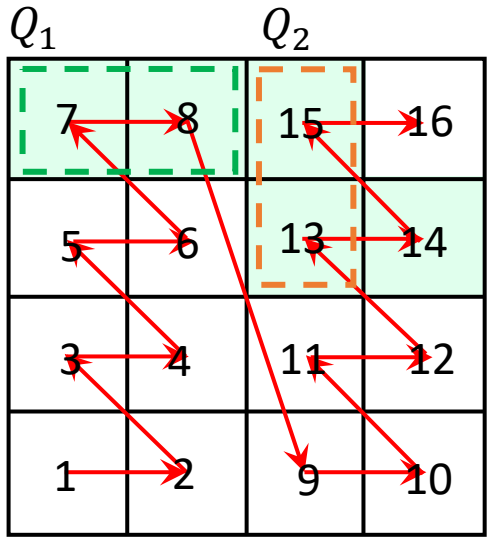
Learning to design SFC

- Design a SFC that combines the advantage of multiple SFCs and thus reach to an optimized performance (**piecewise SFC**)



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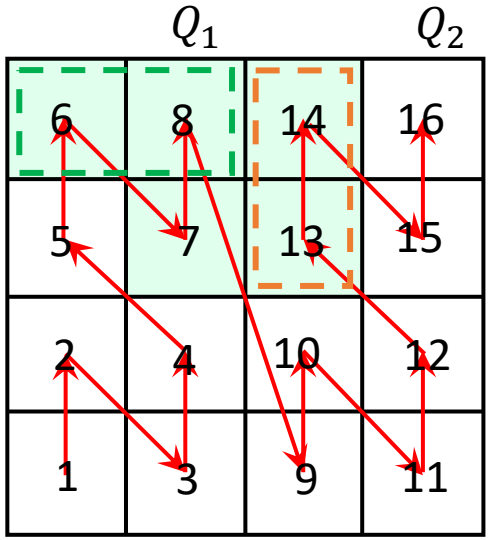
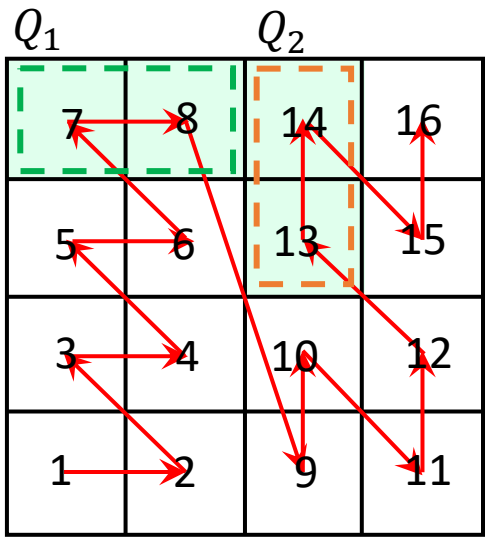


(b) SFC-2 works best for Q_2.



(c) SFC-3 combines SFC-1 and SFC-2, works best for both queries.

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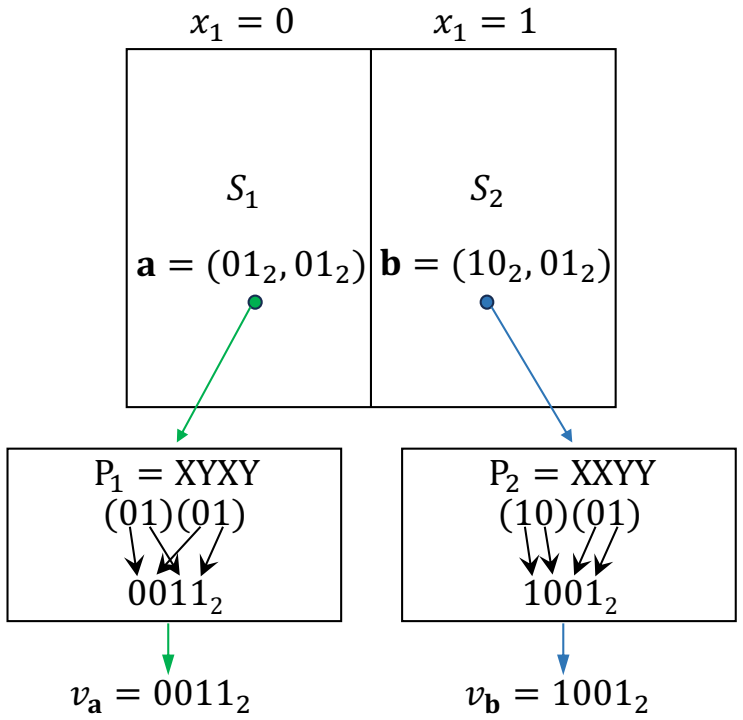
Problem Statement

- Database D
  - Each data point $\mathbf{x} \in D$, has n dimensions, denoted by $\mathbf{x} = (d_1, d_2, \ldots, d_n)$
- Query Workload Q
  - Each query $q \in Q$, $q = (x_{\min}, y_{\min}, x_{\max}, y_{\max})$
- Space-Filling Curve Design for Query Processing
  - Given a database D and a query workload Q, develop a **piecewise SFC**, aiming to optimize the performance of an index built on the SFC values of data points in D.

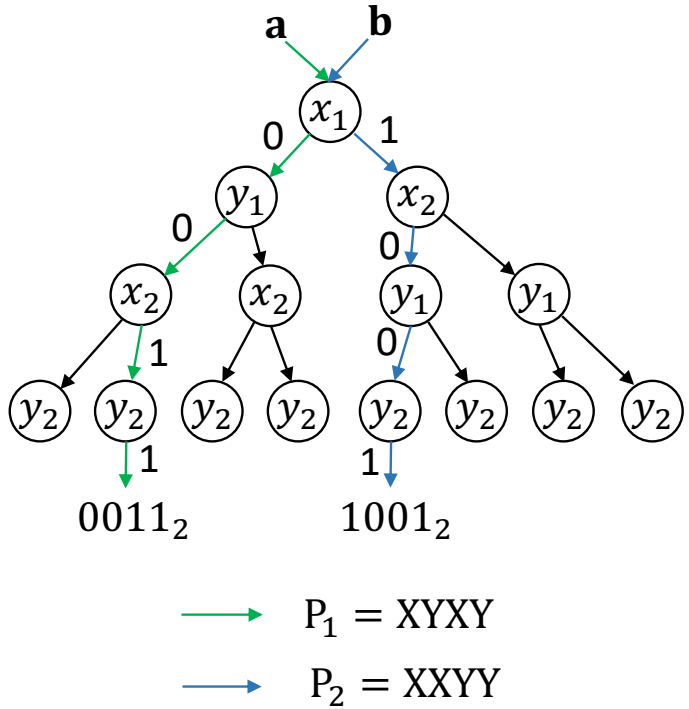
Jiangneng Li et al. **Towards Designing and Learning Piecewise Space-Filling Curves.** VLDB'23

Bit Merging Tree (BM-Tree) Overview

- **BM-Tree:** use **reinforcement to construct a piecewise space filling curve** for better query performance.



(a) Example of Piecewise SFC Design.



(b) Example of BMTree Structure.

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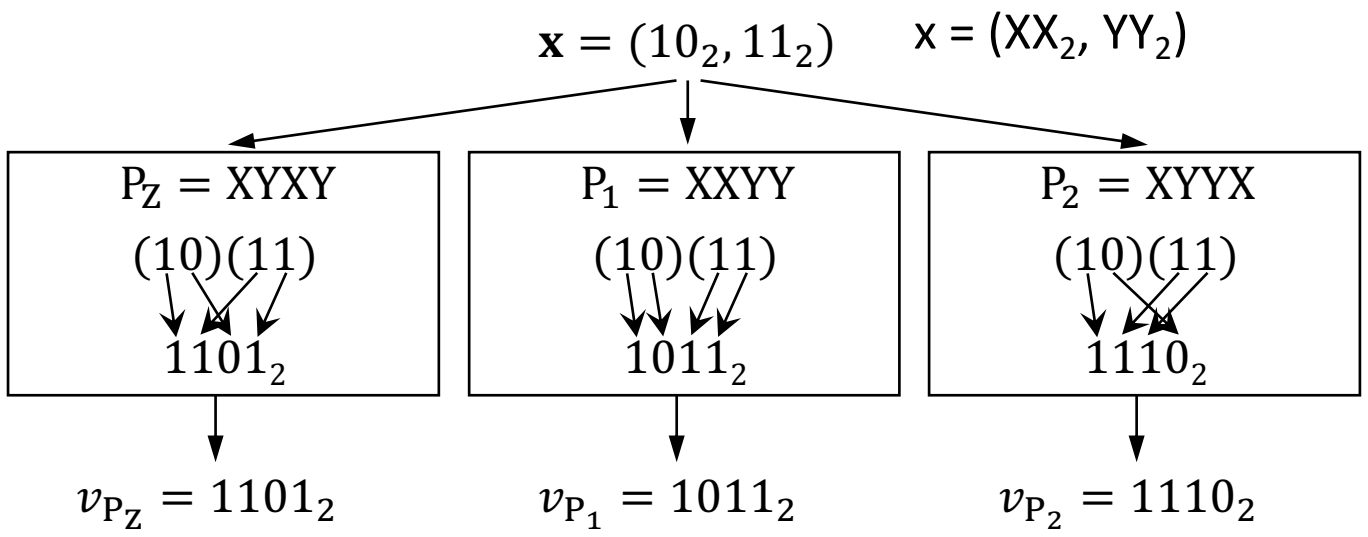
Bit Merging Pattern (BMP)

- The bit merging pattern (BMP, Nishimura & Yokota, SIGMOD'17) describes a set of bit merging-based SFCs.
  - The input data is first written as the binary form, then merge the bit according to the pattern (e.g., XYXY)



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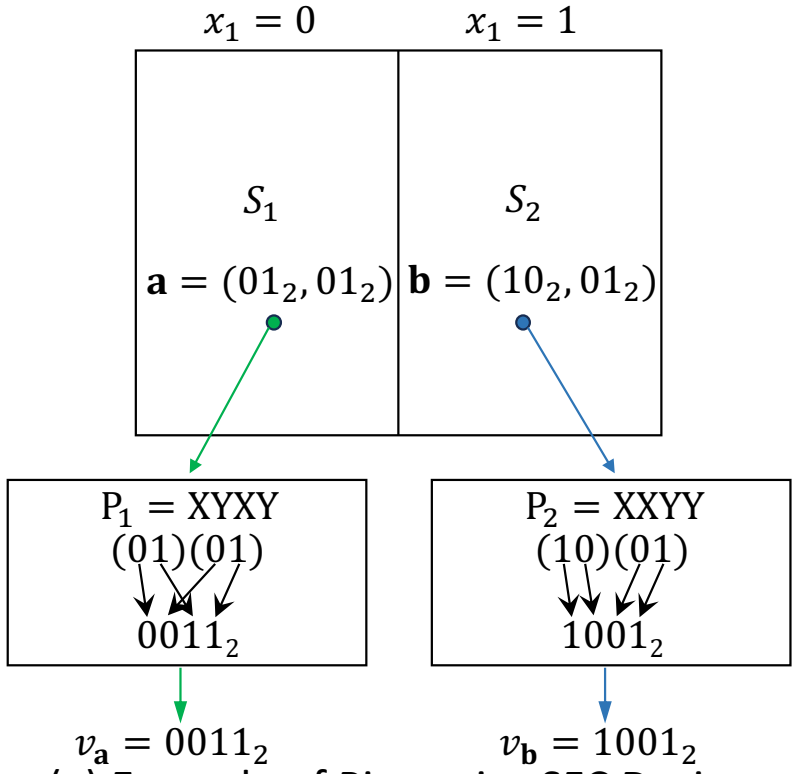
Piecewise SFC Design

- A way of seamlessly integrating the subspace partitioning and BMP generation while ensuring the desired properties.



(a) Example of Piecewise SFC Design.

follow the left-to-right BMP design:

- choose the first bit x_1 for BMP P= X???.
- Then the whole data space is partitioned into two subspaces: Left subspace corresponds to $x_1 = 0$; right $x_1 = 1$
- Then separately design different BMPs for the two subspaces (S_1 and S_2).
- …

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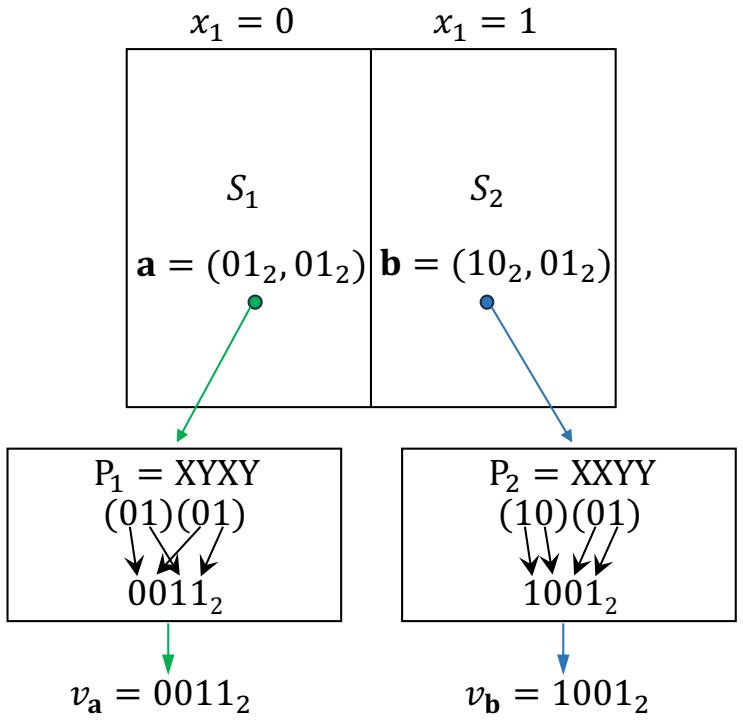
Bit Merging Tree (BMTree)

- The BMTree is to model the partition and BMP design of a piecewise SFC.



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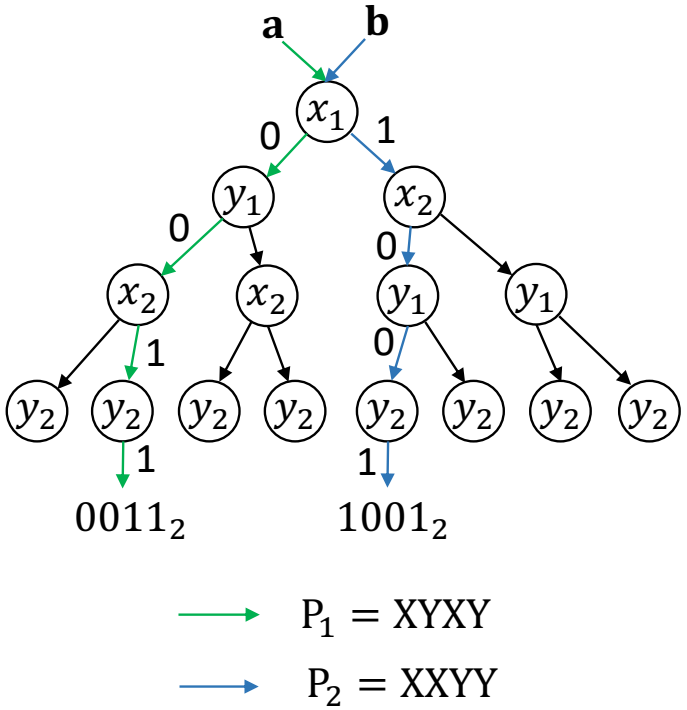
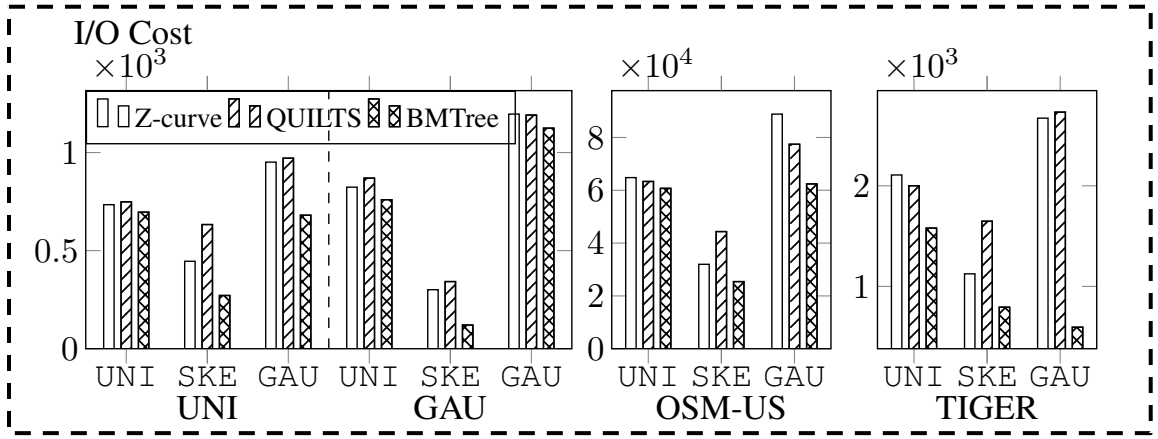


(b) Example of BMTree Structure.

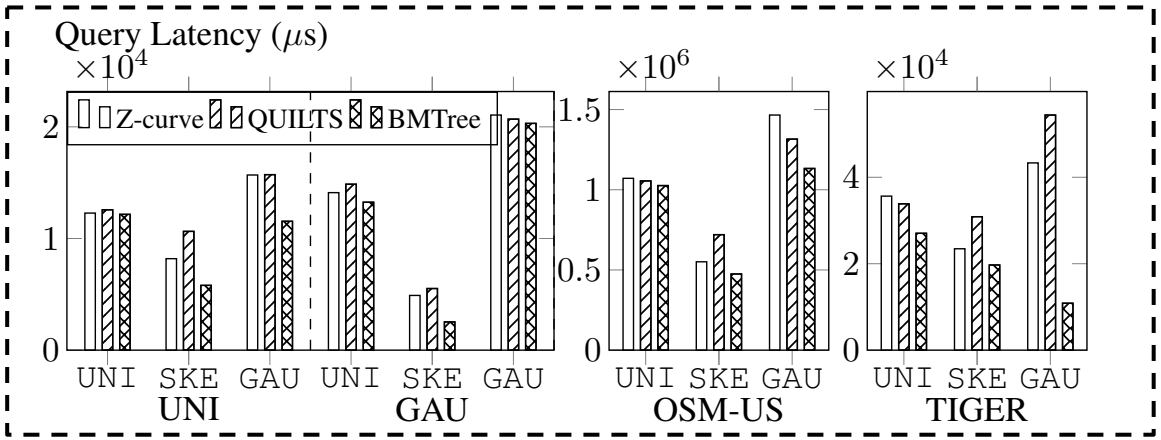
Jiangneng Li et al. **Towards Designing and Learning Piecewise Space-Filling Curves.** VLDB'23

BM-Tree performance

- Experiment on PostgreSQL.



(a) I/O Cost



(b) Query Latency

Jiangneng Li et al. **Towards Designing and Learning Piecewise Space-Filling Curves.** VLDB'23

ML-enhanced Index

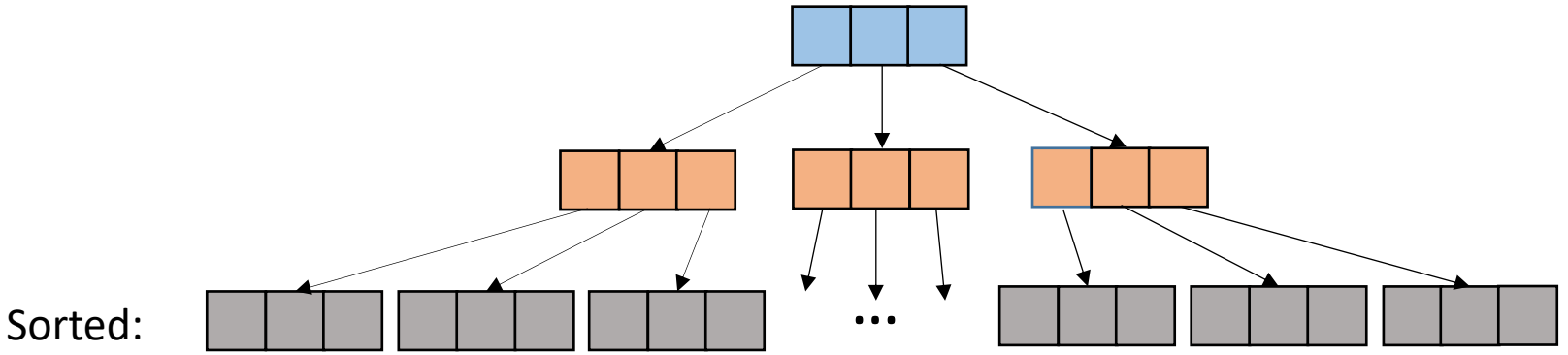
- We will discuss ML-enhanced methods that aid three types of index operations.
- **Insertion**: Building a better index for dynamic data.
  - RLR-tree: learning to improve R-tree insertion
  - BM-tree: learning to design space filling curve
- **Bulk-loading**: Constructing a better index through bulk-loading.
  - PLATON: R-tree packing with learned partition policy
- **Query**: Optimizing index search operation.
  - AI+R-tree: learning to accelerate R-tree search

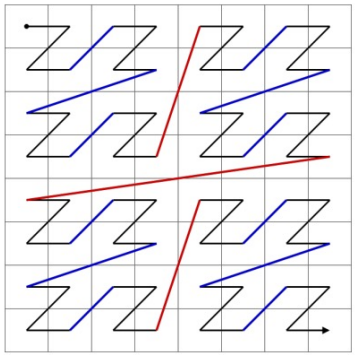
R-tree Bulk-loading/Packing

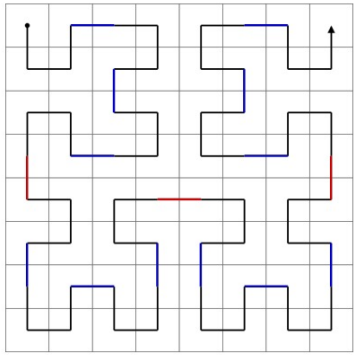
- R-tree packing is usually performed at index construction to build an R-tree with better **space utilization** and **query performance**.
  - **Bottom-up packing**: build the R-tree from leaf nodes upward by sorting the data objects in a heuristic order with a good clustering property.
  - **Top-down packing**: build the R-tree through recursive partitioning, with a partition policy that greedily optimizes a heuristic cost function.
- **The use of heuristic rules results in the constructed R-tree only performing well for certain data distribution and workload patterns.**

Bottom-up R-tree packing

- Bottom-up methods build the R-tree from leaf nodes upward by sorting the data objects in a heuristic order with a good clustering property.



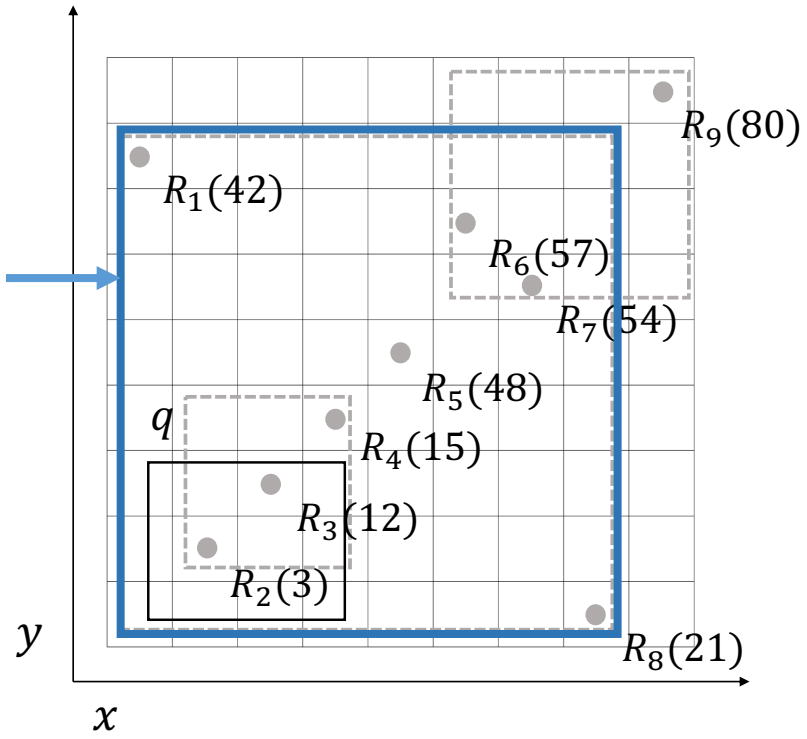




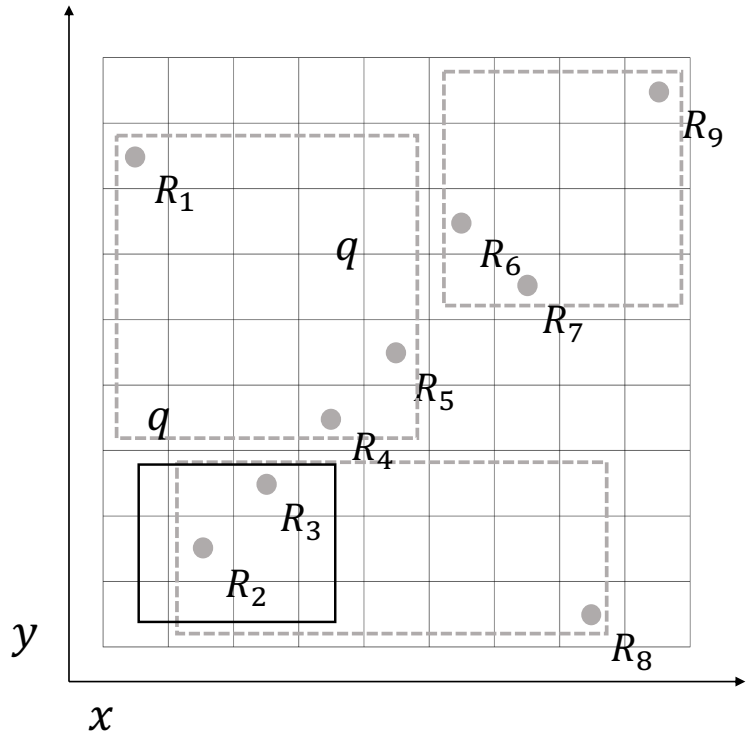
Bottom-up R-tree packing

- Heuristic sort order → only performing well for **certain data distributions and workload patterns**.

Bad nodes spanning a large space



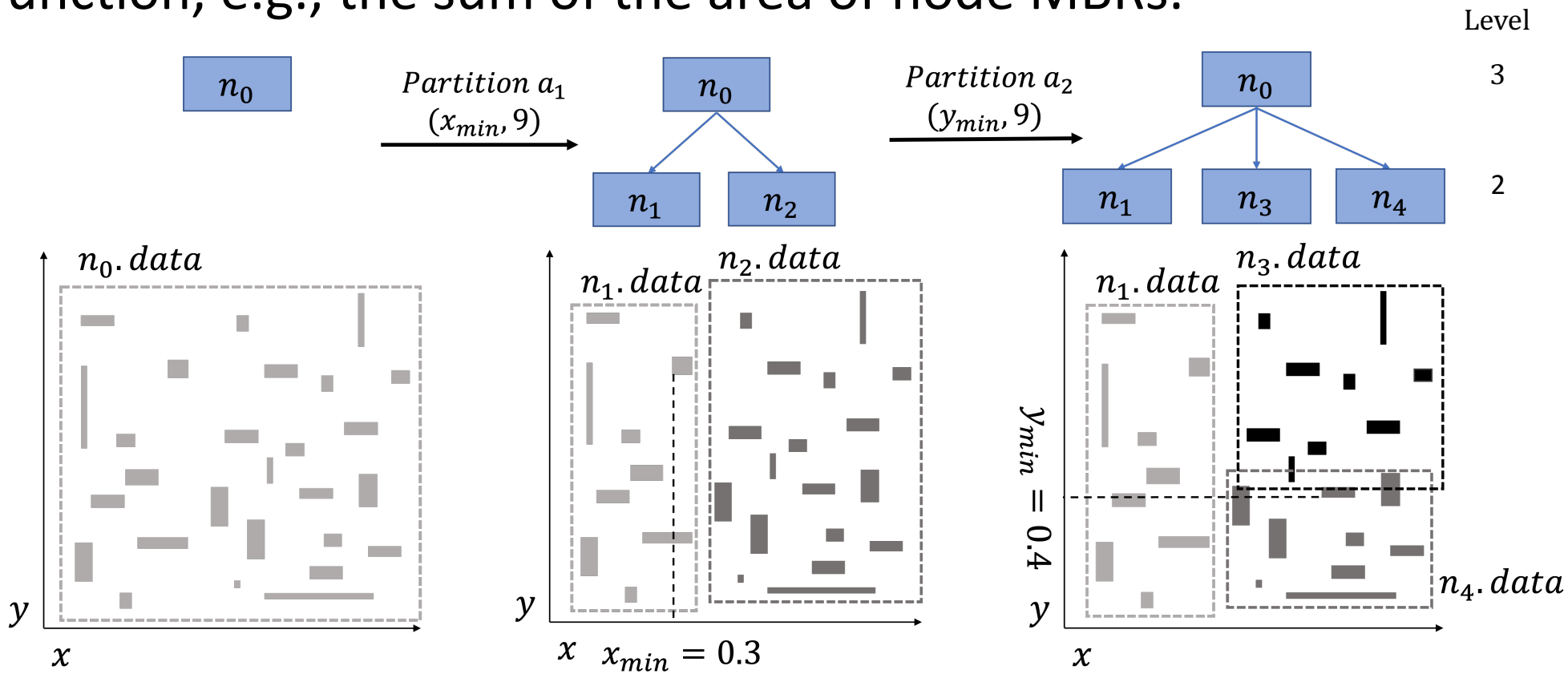
ZR



A better R-Tree

Top-down R-tree packing

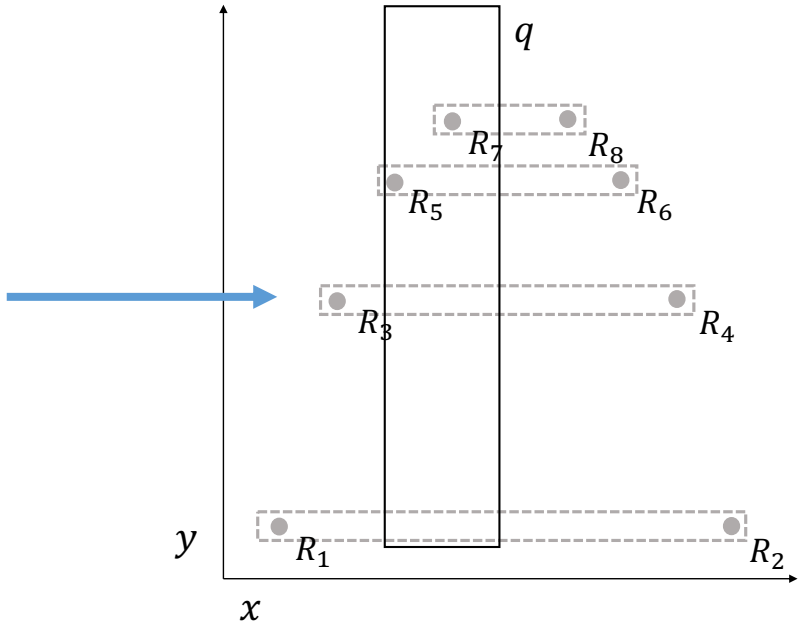
- Top-down methods build the R-tree through recursive partitioning, with a partition policy that greedily optimizes a heuristic cost function, e.g., the sum of the area of node MBRs.



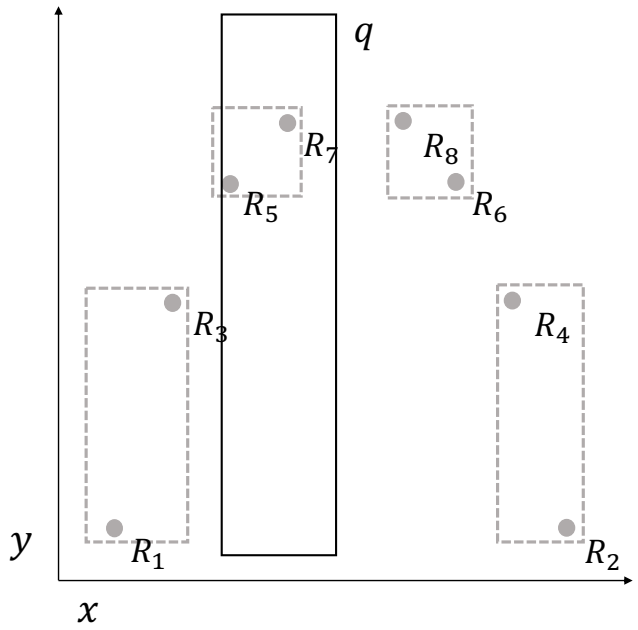
Top-down R-tree packing

- Heuristic cost function → not working well for **different data distributions and workload patterns**.
- The greedy partition policy also **ignores the dependencies** between the partition decisions on different nodes.

Long & thin stripes



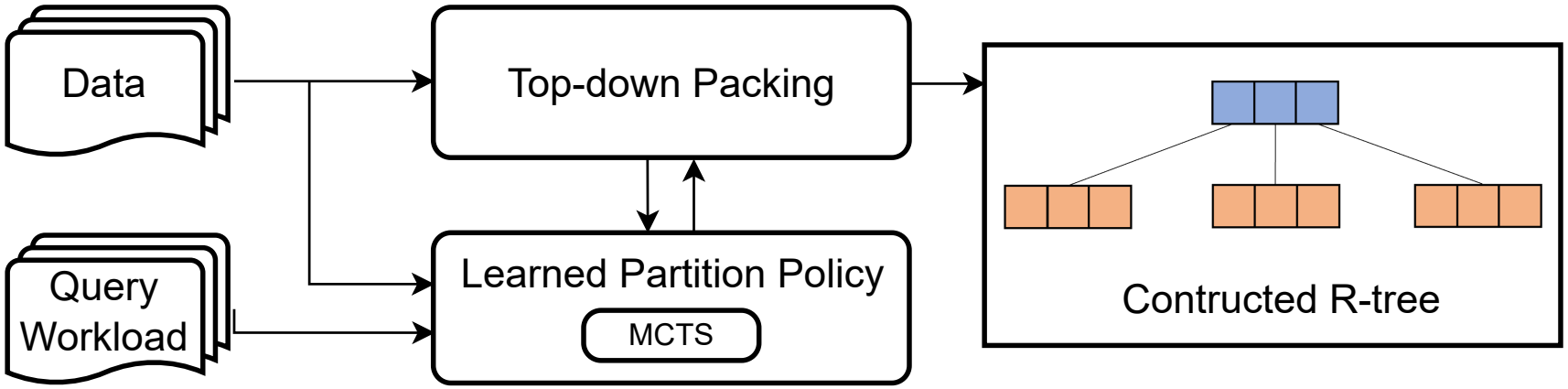
TGS



A better R-Tree

Learning to Pack R-tree

- **PLATON:** use machine learning to **optimize the partition policy** during **top-down packing** for better query performance.
  - PLATON adapts to different data distribution and workload patterns.
  - Light-weight model (Monte Carlo Tree Search) and performance-optimized algorithm



Jingyi Yang et al. **PLATON: Top-down R-tree packing with learned partition policy.** SIGMOD'24

Overview of PLATON

- PLATON is designed with the following goals.
  - Optimizing query performance.

  → Top-down packing as MDP, Monte Carlo Tree Search
  - Designing exploration and simulation strategy for better convergence.

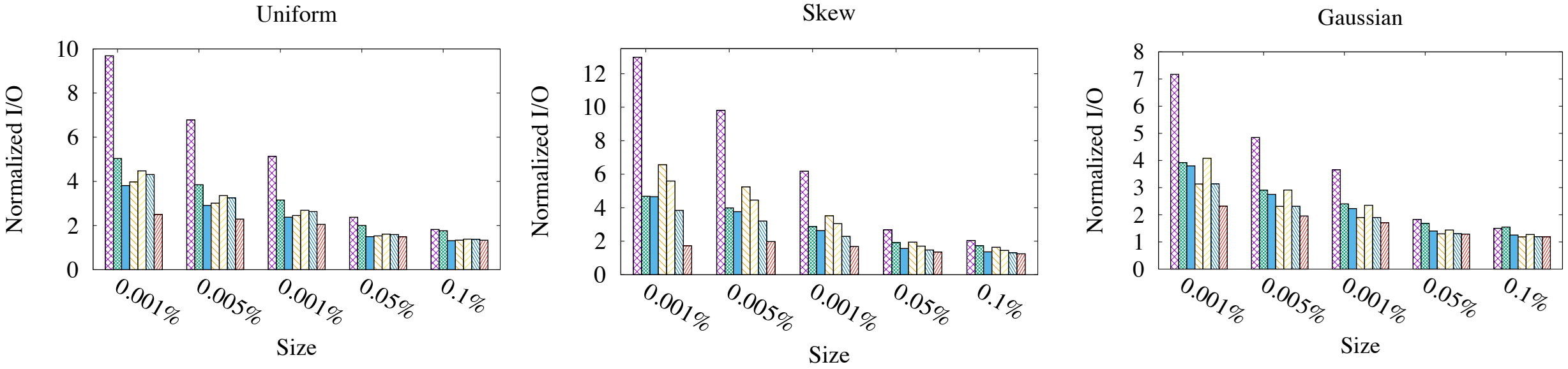
  → Incorporate domain knowledge into MCTS simulation
  - Efficiently learning the partition policy.

  → Divide and conquer strategy, two optimization techniques -> $O(n)$ $training$

Jingyi Yang et al. **PLATON: Top-down R-tree packing with learned partition policy.** SIGMOD'24

Comparison with R-tree variants

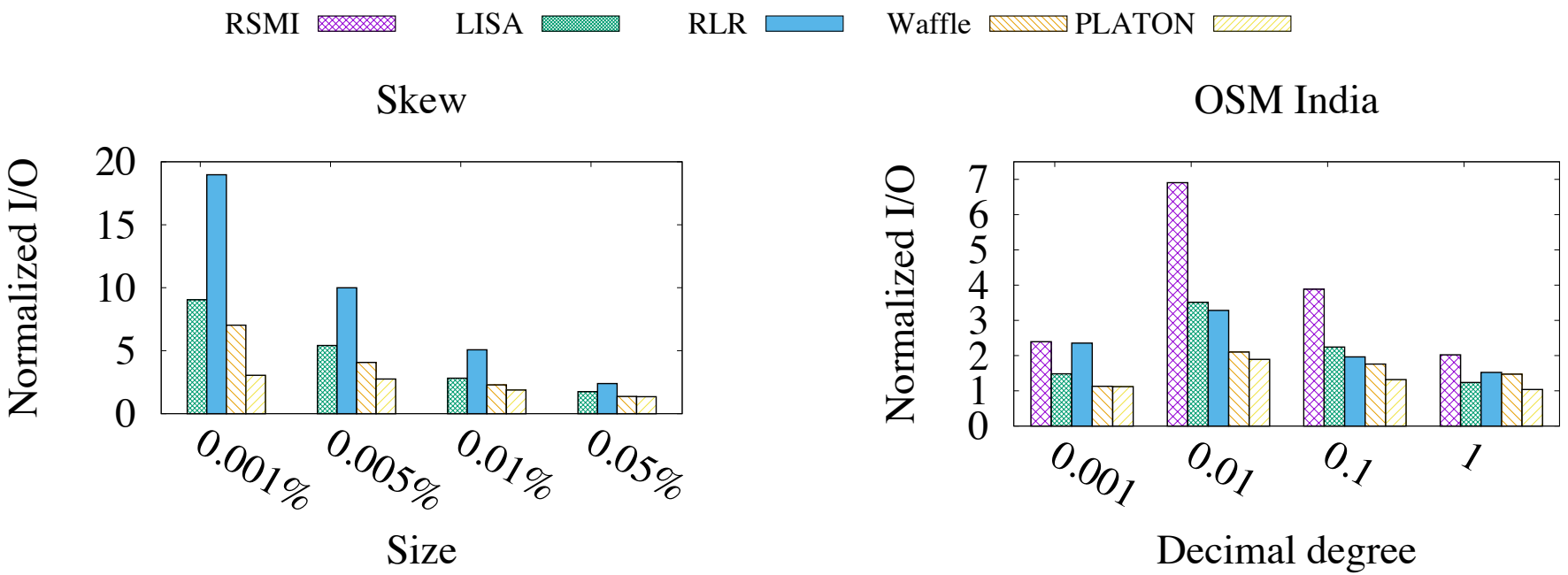
- PLATON significantly outperforms all existing R-tree variants for range query with varying sizes.
- It achieves a speed up of 1.52×, 2.70× and 1.35× compared to the best-performing baseline.



Jingyi Yang et al. **PLATON: Top-down R-tree packing with learned partition policy.** SIGMOD'24

Comparison with learned/workload-aware index

- PLATON achieves a speedup of up to 2.30× and 1.42× compared to the best performing baseline Waffle.



Jingyi Yang et al. **PLATON: Top-down R-tree packing with learned partition policy.** SIGMOD'24

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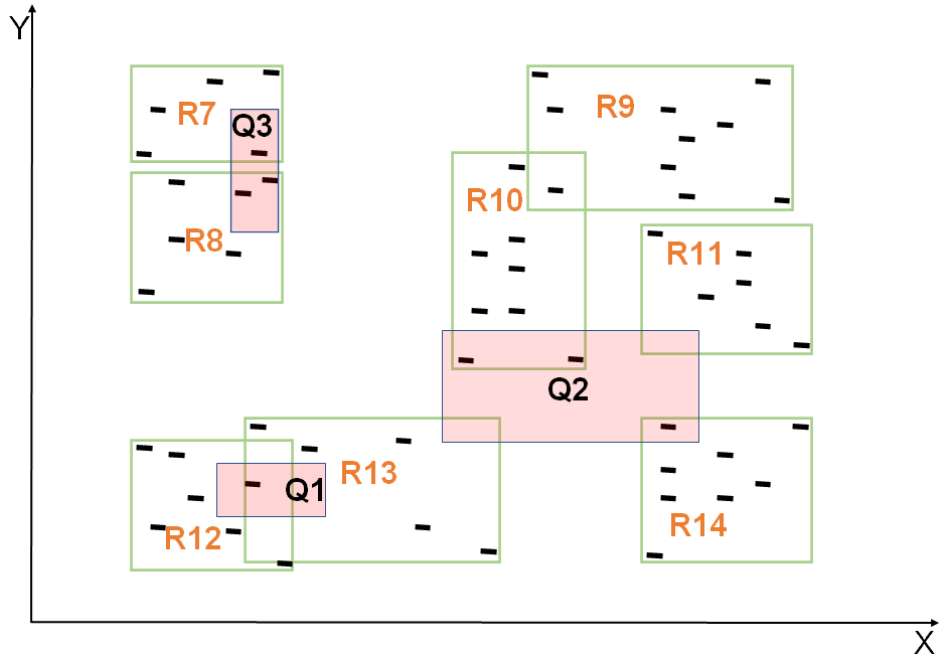
- **Query**: Optimizing index search operation.
  - AI+R-tree: learning to accelerate R-tree search

R-Tree Search

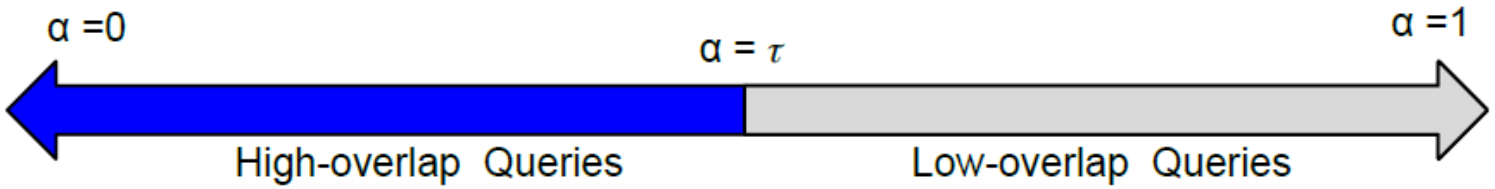
- In the R-tree, objects are stored using Minimum Bounding Rectangles (MBRs), and the MBRs of tree nodes can overlap in space.
- A query would access all leaf nodes with overlapping MBR, and some queries may access many extraneous node.
- **The excessive number of extraneous nodes accessed by high-overlap queries leads to high I/O cost.**



Query	Visited leaf nodes	True leaf nodes
Q1	R12, R13	R12
Q2	R10, R11, R13, R14	R10, R14
Q3	R7, R8	R7, R8

Overlap Ratio

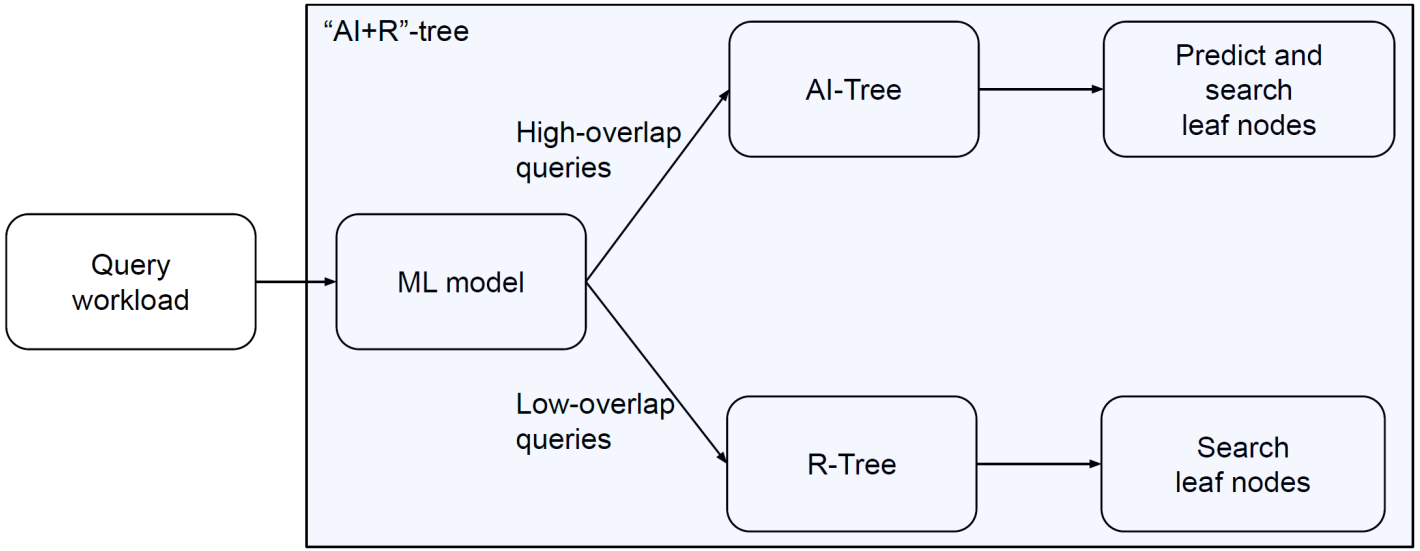
- Define an overlap ratio α to quantify the degree of extraneous leaf node accesses required by a range query.
- For a range query:
  - $\alpha = \frac{Number\ of\ true\ leaf\ nodes\ that\ actually\ contains\ the\ output\ data\ objects}{Number\ of\ leaf\ nodes\ searched\ by\ the\ R{-}Tree}$
  - α is in the range [0,1]
- High-overlap Queries:
  - A range query is declared as a "high-overlap query" if the value of α is less than a pre-defined threshold τ.



Mamun et al. **The "AI+R" tree: An instanced optimized R-tree.** MDM'22

AI+R-Tree: learning to accelerate R-tree search

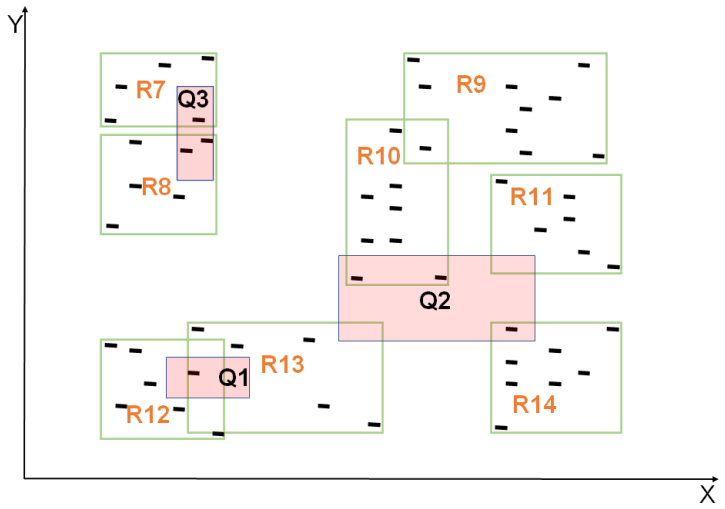
- Leveraging a binary classifier to automatically differentiate between high- and low-overlap queries.
- Process the high-overlap queries using the AI-tree.
- Process the low-overlap queries using the R-tree.



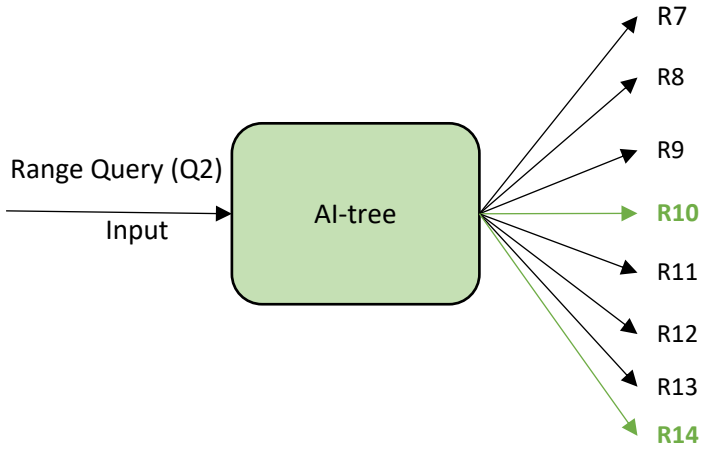
Mamun et al. **The "AI+R" tree: An instanced optimized R-tree.** MDM'22

AI+R-Tree: learning to accelerate R-tree search

- AI-Tree: predicting the node id that contains qualifying data objects
- Improve prediction accuracy with multiple space-partitioned models



An example of leaf nodes in an R-tree



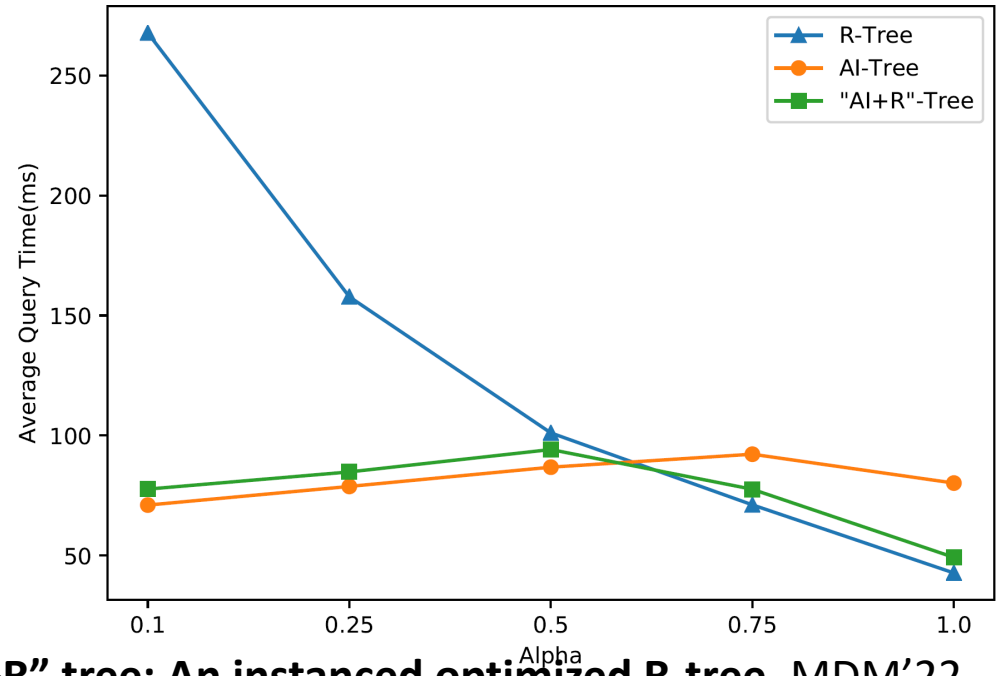
Total number of classes > 2
For an input, the number of output classes ≥ 0

M1 Q1	M2	M3	M4
M5	M6	M7	M8
M9	M10 Q2	M11	M12
M13	M14	M15	M16

Mamun et al. **The "AI+R" tree: An instanced optimized R-tree.** MDM'22

AI+R-Tree: learning to accelerate R-tree search

- For the high-overlap queries, the AI-tree performs better.
- For the low-overlap queries, the traditional R-tree performs better.
- The combined AI+R tree have more consistent performance.



Mamun et al. **The "AI+R" tree: An instanced optimized R-tree.** MDM'22

Summary

- ML-enhanced indexes are motivated by the need for more robust and generalizable learning-based indexes.

- Many of the index organization policies (implicitly) involve the use of heuristic rules, which can be formulated into a decision problem and optimized with ML/RL.
  - Node choosing and splitting policy in a multi-dimensional R-tree index
  - Data partition policy underlying a space-filling curve
  - Data sorting/partition policy in index bulk-loading

- Using Machine Learning model as “shortcuts” for inefficient operations.

ML4DB Paradigms

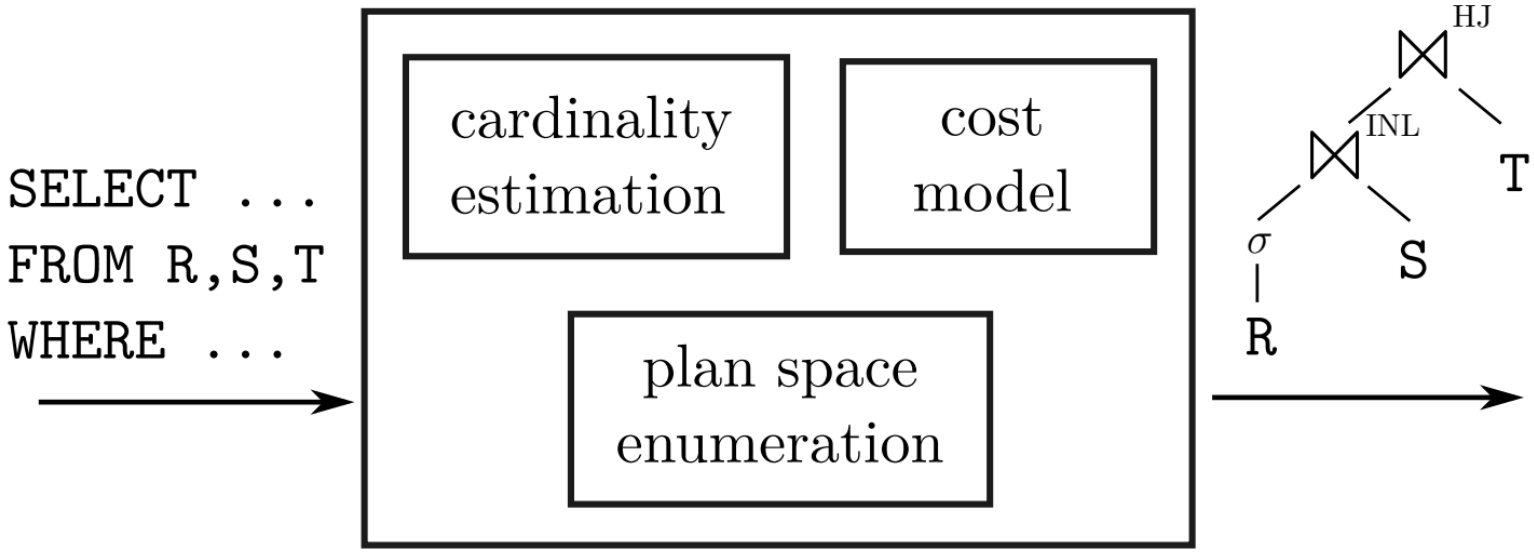
- We study ML4DB paradigms in the context of two important problem
  - Database indexing
  - Query optimization

ML4DB Paradigms in Query Optimization

- Part 1: Preliminary
- Part 2: Learned query optimizer
- Part 3: ML-enhanced query optimizer
- Part 4: Summary

Query optimizer

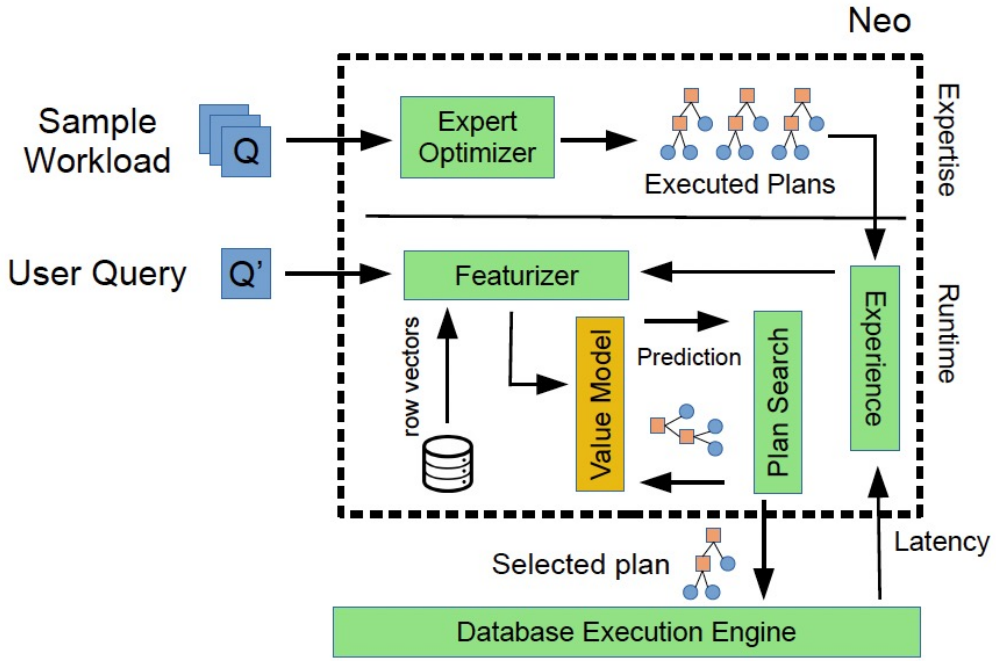
- A traditional database query optimizer consists of three components
  - Cardinality estimation: histogram
  - Cost estimation: formula-based
  - Plan enumeration: dynamic programming



Victor Leis et al. **How Good Are Query Optimizers, really?** VLDB'15

Learned query optimizer: NEO

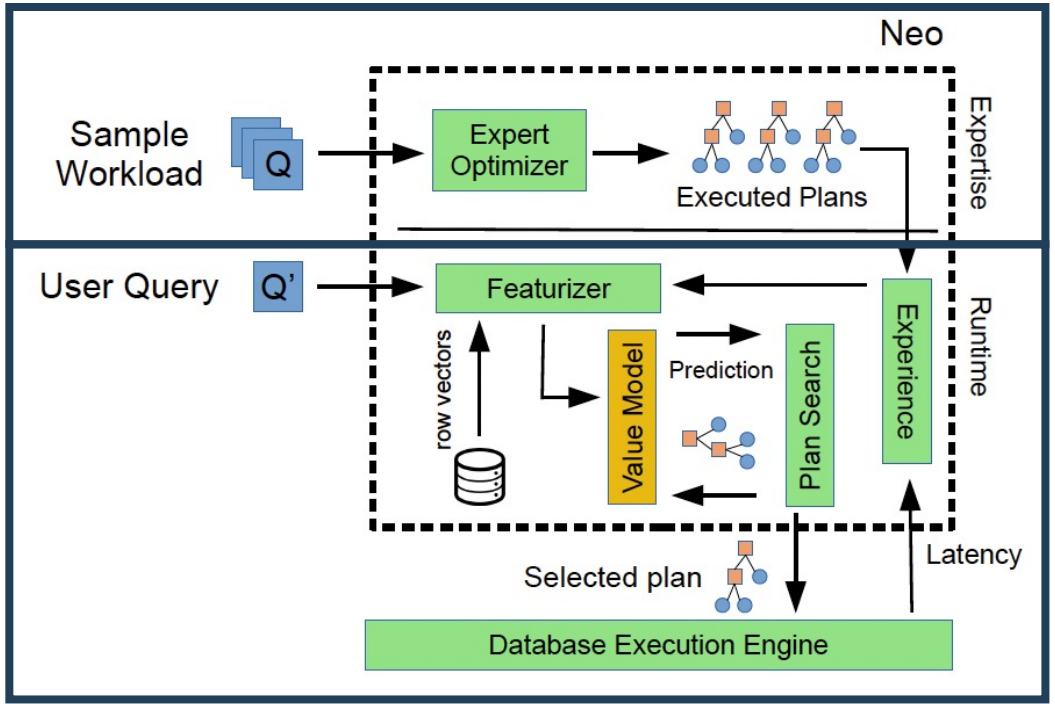
- Motivation: Query optimizers require a great deal of hand-tuning for specific workloads and datasets.
- NEO: Tailor the query optimizer to user's DB instance and workloads.



Ryan Marcus et al. **NEO: a learned query optimizer.** SIGMOD'19

Learned query optimizer: NEO

- Two phases
  - Initial phase: Learn a value network from an expert optimizer
  - Runtime phase: Plan search guided by the value network

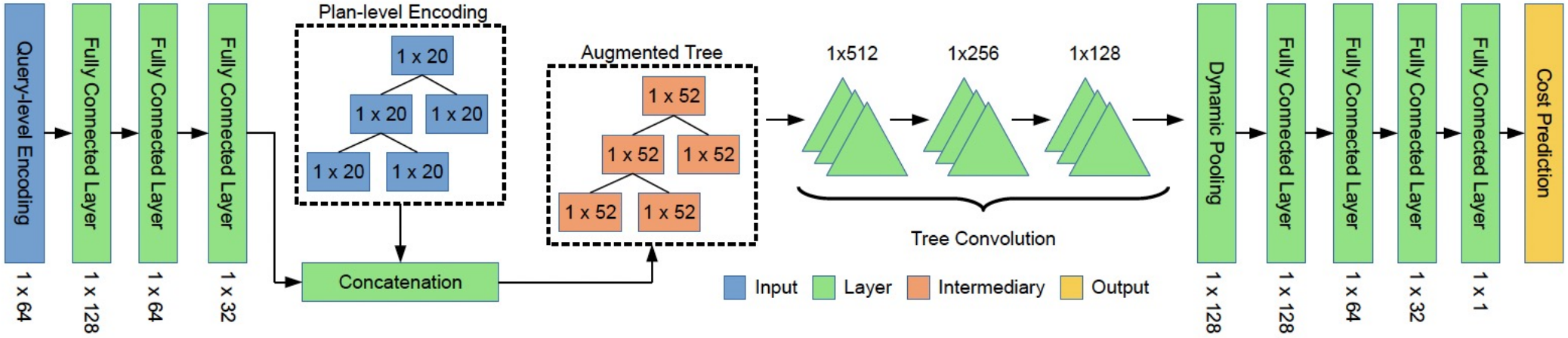


Ryan Marcus et al. **NEO: a learned query optimizer.** SIGMOD'19

Value Network

- Given a partial execution plan P_i, the value network predicts the best-possible query latency achievable by a complete execution plan P_f such that $P_i \subset P_f$

$$M(P_i) \approx \min\{C(P_f) \mid P_i \subset P_f \wedge P_f \in E\}$$



Ryan Marcus et al. **NEO: a learned query optimizer.** SIGMOD'19

Value network guided plan search

- Initialize an empty min heap to store partial execution plans
- Add partial execution plan with an unspecified scan for each relation into the heap
- At each search iteration
  - Remove the subplan P_i at the top of the min heap
  - Enumerate $P_i's$ Children, score them with the value network, add to heap
- Terminate when a complete plan is found, or when a time threshold is reached

Learned query optimizer: NEO

- Revisit the three components in NEO
  - Cardinality estimation: Tree convolution neural network (implicit)
  - Cost estimation: Tree convolution neural network
  - Plan enumeration: value network guided search

- The three components are jointly optimized in an end-to-end reinforcement learning pipeline.

Motivation of ML-enhanced query optimizer

- **Robustness**
  - Cold start problem: the performance of the model largely depends on the amount and diversity of training query plans, which are costly to gather
- **Complexity**
  - Huge plan space, hard to optimize, long training time
- **Generalization Capability**
  - Type of query: Select-Project-Join (SPJ) only
  - Learning-based optimizers are trained on a specific database with specific hardware and software configuration

- Can we improve the query optimizer without getting rid of the expert query optimizer in existing databases, e.g. PostgreSQL?

ML-enhanced Query Optimizer

- We will discuss three types of ML-enhanced query optimizer.

- **Bandit Optimizer**: Learning to steer query optimizer through hint-set.
- **Lero**: A Learning-to-Rank Query Optimizer
- **ParamTree**: Learning hyperparameters for formula-based cost model.

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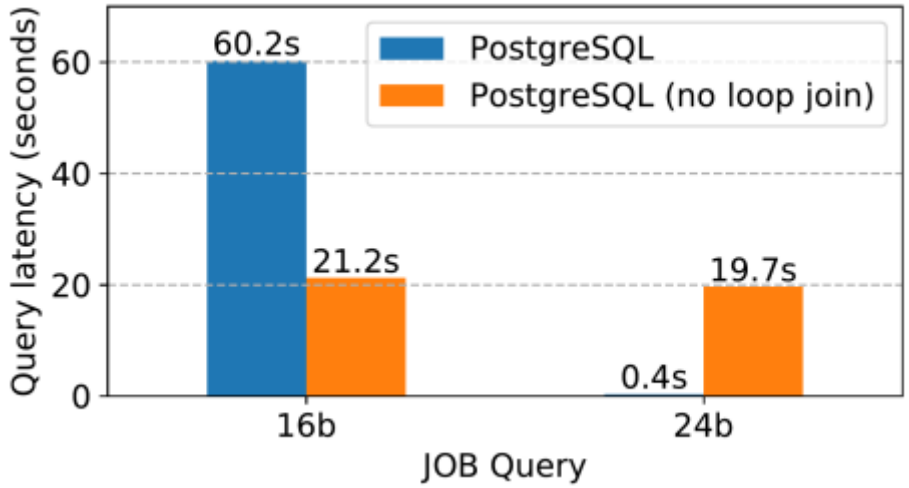
Bandit Optimizer

- Observation: Coarse-grained hints can improve the performance for certain types of queries
- Example: Cardinality under-estimates frequently prompt the query optimizer to select loop joins when other methods (merge, hash) would be more effective



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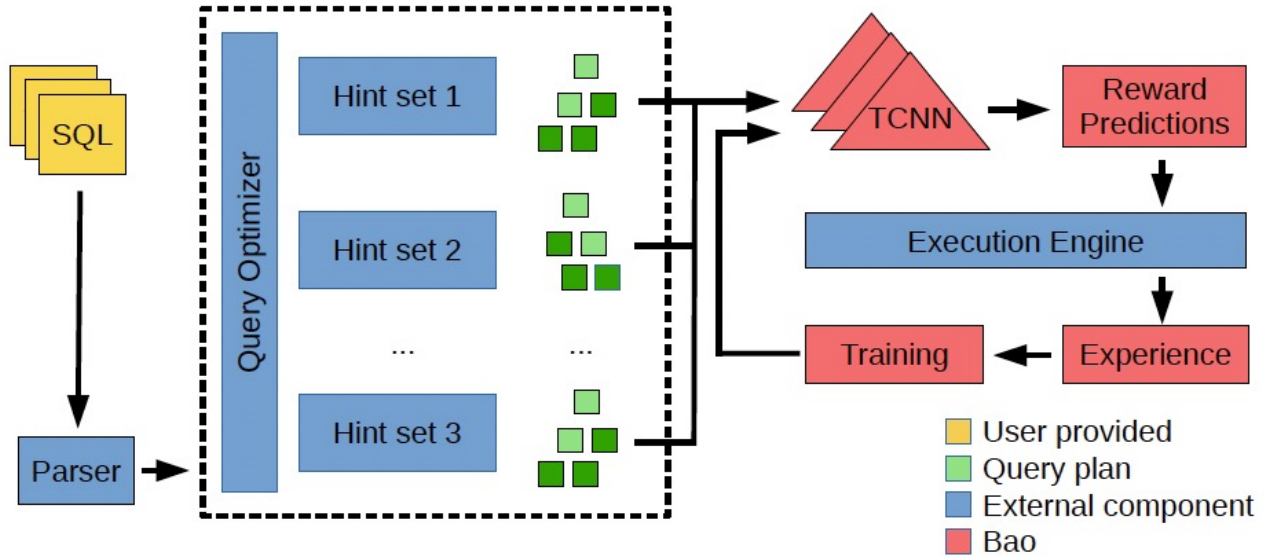
Bandit Optimizer

- Offload alternative plan enumeration
  - Only consider the best plan generated by expert optimizer for a hint set
- Model Plan Selection as a Contextual Multi-armed bandit



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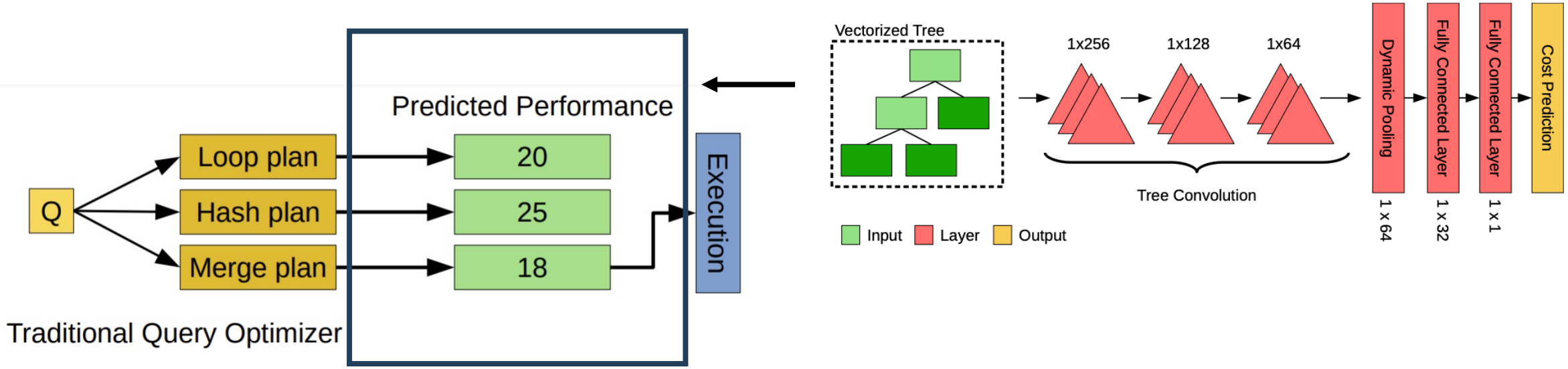
Enumerate Query Hints

- Query Hint Set: A combination of configuration knobs
- Query plans are enumerated using different query hint sets
- Bao determines the optimal hint with a Tree CNN based predictive model



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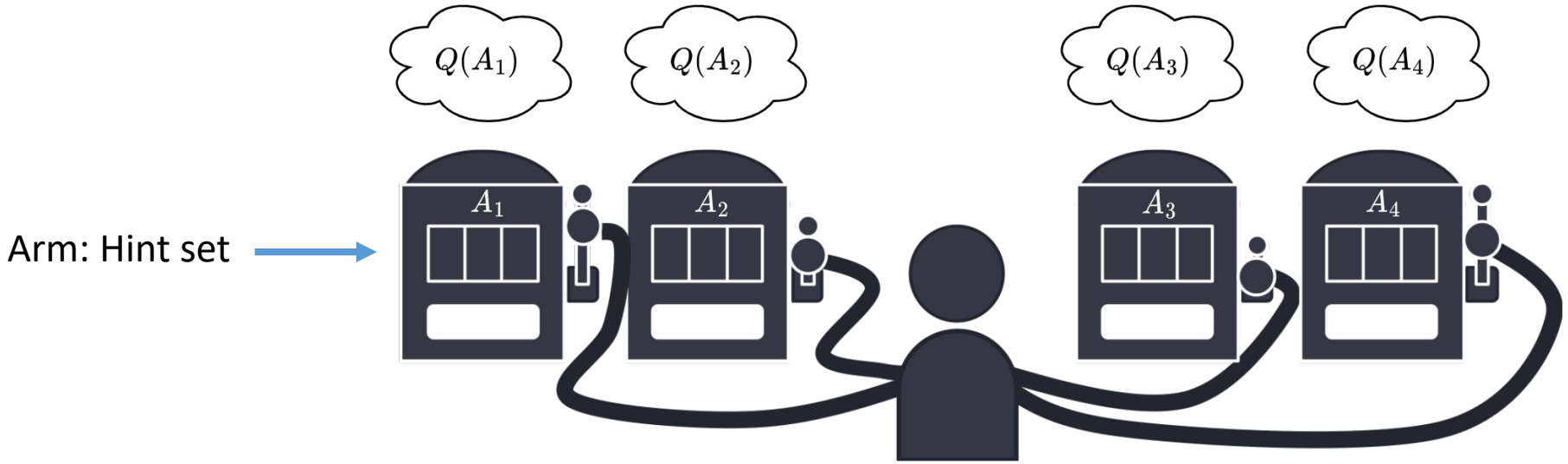
Contextual Multi-armed bandit

- Context: The set of query plans produced by the underlying optimizer given each hint set
- Exploration-exploitation tradeoff



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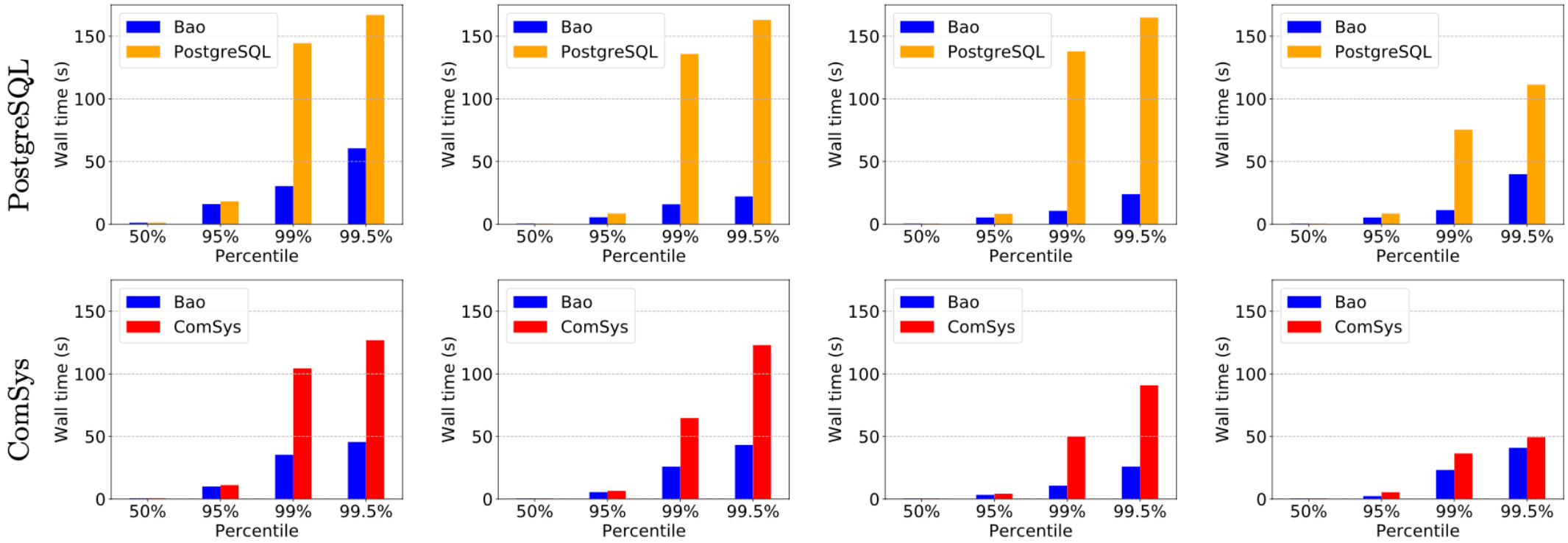
Bandit Optimizer

- BAO drives significant improvement in runtime, especially at tail



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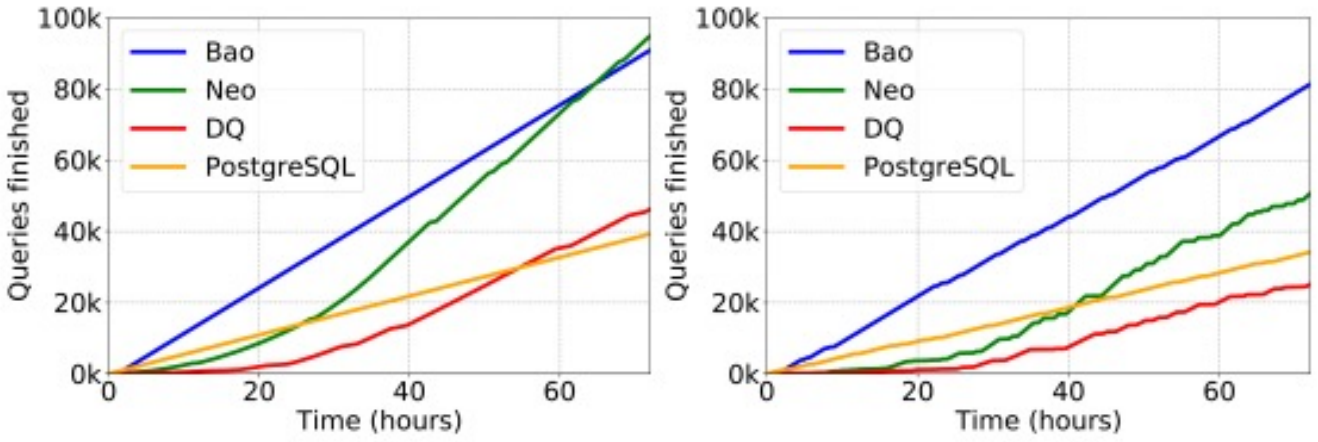
Bandit Optimizer

- With a stable workload, BAO converges much faster than NEO
- BAO better adapts to change compared to learned query optimizers



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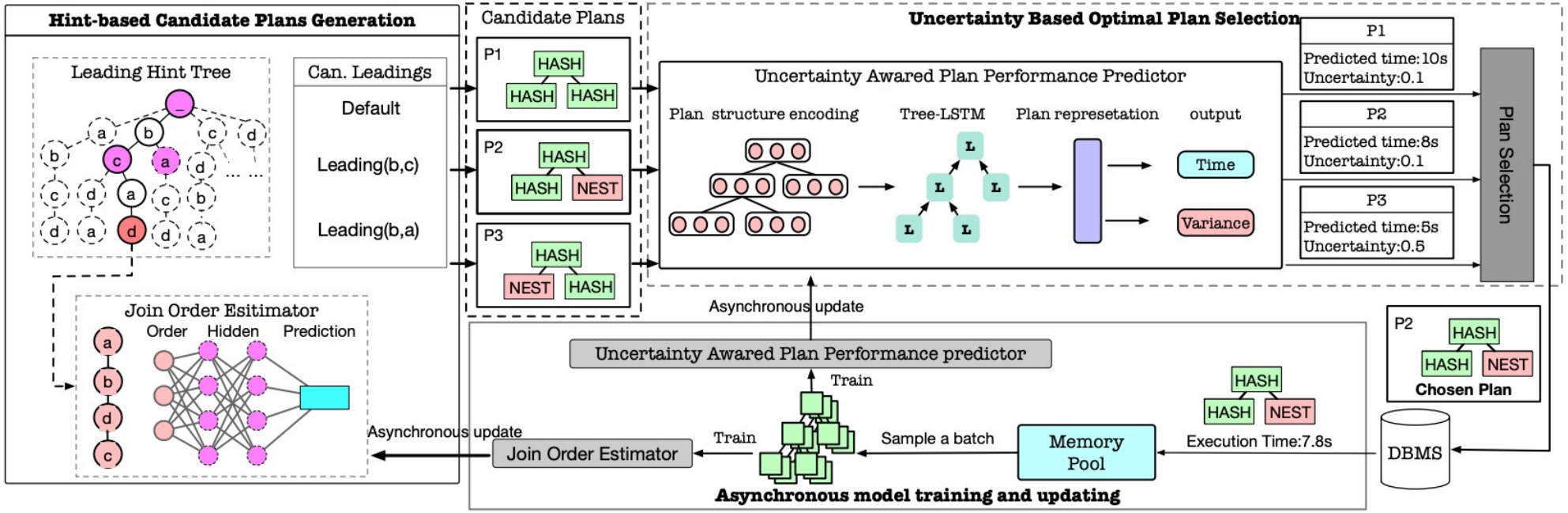
Bandit Optimizer

- Revisit the three components in BAO
- Cardinality estimation: not needed
- Cost estimation: Tree CNN
- Plan enumeration: hint set + Expert query optimizer

Hybrid Query Optimizer - HYBRIDQO

- Select leading hint through machine learning, i.e. MCTS
- Uncertainty based model for plan selection



Xiang Yu et al. **Cost-based or Learning-based? A Hybrid Query Optimizer for Query Plan Selection.** VLDB'23

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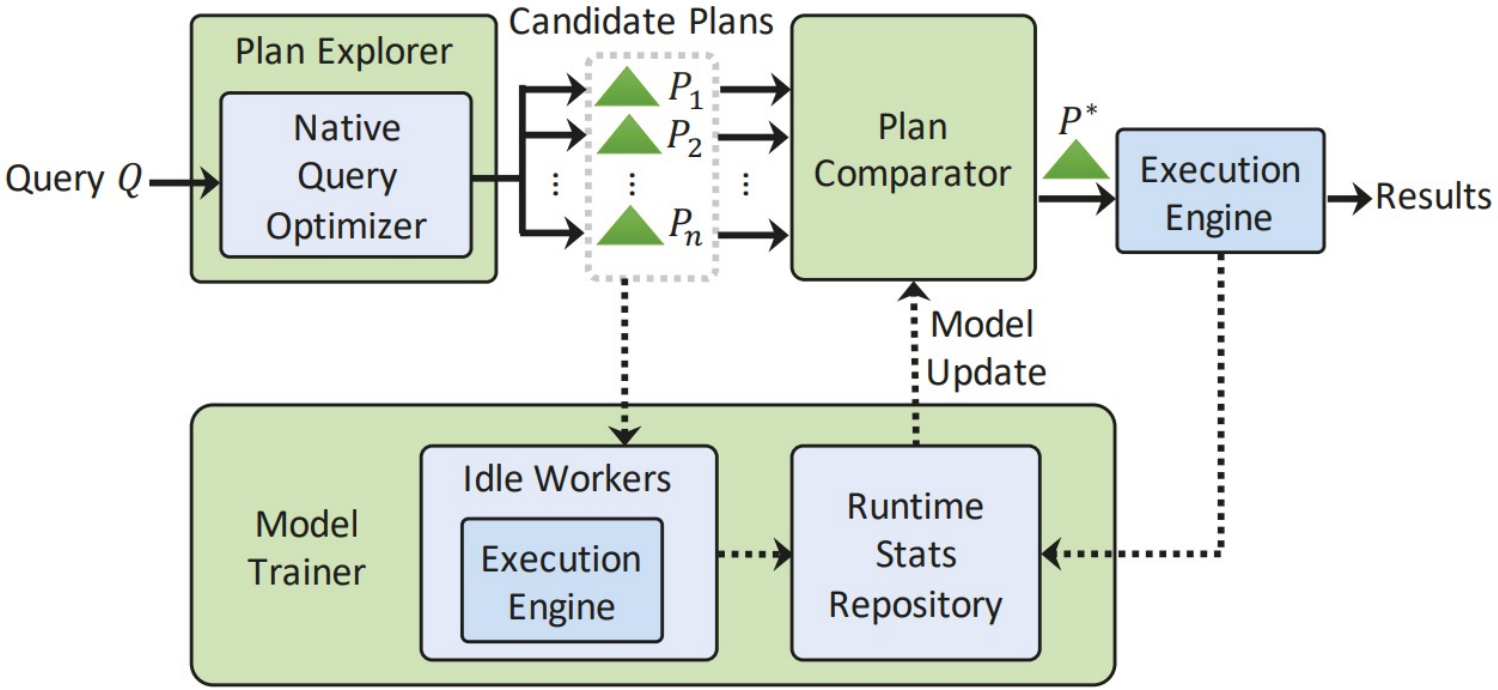
Lero: Learning to Rank Plans

- Lero enumerate candidate plans by adjusting subplan cardinalities
- Using a pairwise plan comparator model to choose the best plan

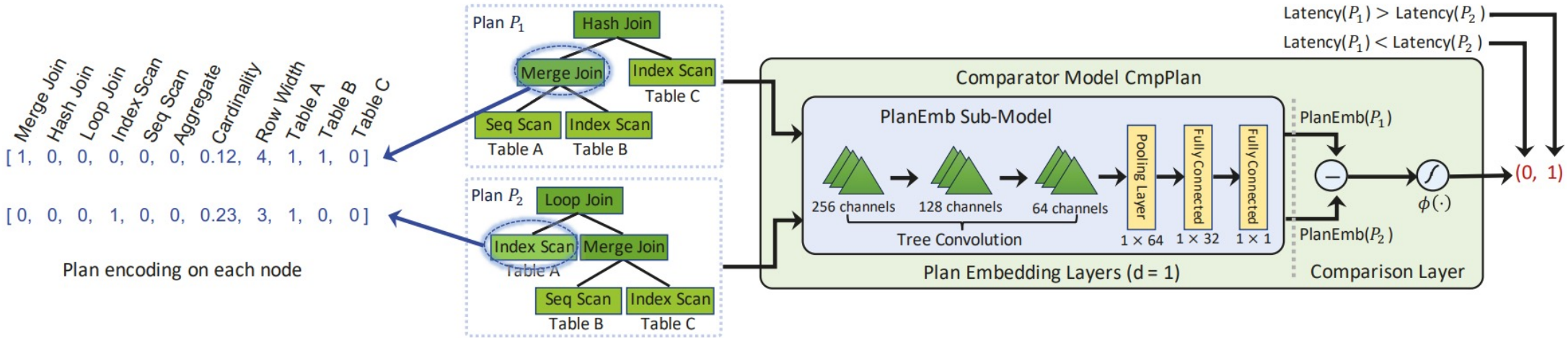


Rong Zhu et al. **Lero: A Learning-to-Rank Query Optimizer.** VLDB'23

Lero: Learning to Rank Plans

- Plan Comparator Model

$$CmpPlan(P_1, P_2) = \begin{cases} 0 \; if \; Latency(P_1) < Latency(P_2) \\ 1 \; if \; Latency(P_1) > Latency(P_2) \end{cases}$$



Rong Zhu et al. **Lero: A Learning-to-Rank Query Optimizer.** VLDB'23

Cardinality as Knob for Plan Explorer

- Lero explore plans by adjusting the sub-plan cardinalities
- Advantages of tuning cardinality:
  - Cardinality directly affect the query plan, introduce diversity
  - Platform-independent

Algorithm plan_explorer(Q, α, Δ)

1: Priority queue candidate_plans $\leftarrow \varnothing$
2: **for** each $f \in F_\alpha^\Delta$ in the increasing order of $|\log f|$ **do**
3: **for** $k \leftarrow 1$ to q (the number of tables in Q) **do**
4: **Inside query optimizer:** let $\mathrm{C}()$ be the default cardinality estimator in native query optimizer
5: $\widetilde{\mathrm{C}}(Q') \leftarrow f \cdot \mathrm{C}(Q')$ for size-k sub-queries $Q' \in \mathrm{sub}_k(Q)$
6: $\widetilde{\mathrm{C}}(Q') \leftarrow \mathrm{C}(Q')$ for sub-queries $Q' \in \mathrm{sub}(Q) - \mathrm{sub}_k(Q)$
7: feed cardinality $\widetilde{\mathrm{C}}()$ into the cost model to generate a plan P
8: candidate_plans $\leftarrow$ candidate_plans $\cup \{P\}$
9: **return** candidate_plans

Rong Zhu et al. **Lero: A Learning-to-Rank Query Optimizer.** VLDB'23

ML-enhanced Query Optimizer

- We will discuss three types of ML-enhanced query optimizer.

- **Bandit Optimizer**: Learning to steer query optimizer through hint-set.
- **Lero**: A Learning-to-Rank Query Optimizer.
- **ParamTree**: Learning hyperparameters for formula-based cost model.

Formula-based cost model

- **Formula-based cost model**: empirical formulas summarized by database researchers and developers over a long time.
- These formulas reflect how a database system interacts with the operating system and hardware components such as memory, CPU, and disk.
- Formula-based cost models typically require database administrators (DBAs) to tune certain hyperparameters (e.g., ratio to normalize I/O and CPU cost)

Jiani Yang et al. **Rethinking Learned Cost Models: Why Start from Scratch?** SIGMOD'24

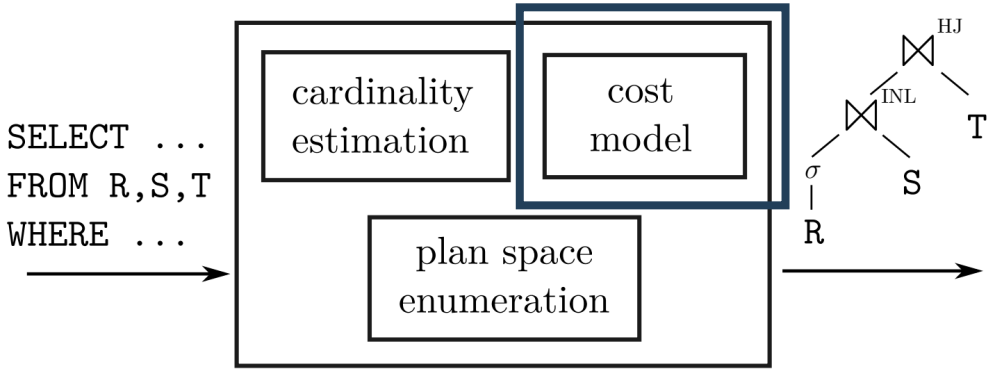
Formula-based cost model

Operator	Cost Type	Cost Formula	
SeqScan	startup_cost	0	
	runtime_cost	cpu	$(r_t + r_o \times N_{qp}) \times tuples\_num$
		disk	$r_s \times table\_pages$
IndexOnlyScan	startup_cost	$\lceil \log_2 index\_tuples \rceil \times r_o + (index\_tree\_height + 1) \times 50 \times r_o$	
	runtime_cost	cpu	$indexSelectivity \times index\_tuples \times (r_t + r_i + r_o \times N_{cp})$
		disk	$\lceil indexSelectivity \times index\_pages \rceil \times r_r$
IndexScan	startup_cost	$\lceil \log_2 index\_tuples \rceil \times r_o + (index\_tree\_height + 1) \times 50 \times r_o$	
	runtime_cost	cpu	$indexSelectivity \times index\_tuples \times (r_i + r_o \times N_{cp} + r_t + r_o \times N_{qp})$
		disk	$\lceil indexSelectivity \times index\_pages \rceil \times r_r + max\_IO\_cost +$ $indexCorrelation^2 \times (min\_IO\_cost - max\_IO\_cost)$ $(max\_IO\_cost = r_r \times \Phi_{Mackert-lohman},$ $min\_IO\_cost = (\lceil indexSelectivity \times table\_pages \rceil - 1) \times r_s + r_r)$
Sort	startup_cost	cpu	$C_t^L + 2 \times r_o \times tuples\_num \times \log_2 tuples\_num$
		disk	**When input_bytes > work_mem:** $2 \times \lceil \frac{input\_bytes}{BLCKSZ} \rceil \times \max(1, \lceil log_{mergeorder} \frac{input\_bytes}{c_w} \rceil) \times (0.75 r_s + 0.25 r_r)$
	runtime_cost	cpu	$r_o \times tuples\_num$
HashJoin	startup_cost	cpu	$C_s^L + C_T^R + R_r \times (r_o \times N_{cp} + r_t)$
		disk	$\text{sgn}(nbatches - 1) \times (r_s \times P_r)$
	runtime_cost	cpu	$C_t^L - C_s^L + r_o \times N_{cp} \times R_l + N_{cp} \times r_o \times R_l \times R_r \times innerbucketsize \times 0.5$ $+R_o \times (r_t + r_o \times N_{qp})$
		disk	$\text{sgn}(nbatches - 1) \times (r_s \times (P_r + 2 \times P_l))$

Jiani Yang et al. **Rethinking Learned Cost Models: Why Start from Scratch?** SIGMOD'24

ParamTree: Learned formula-based cost model

- **Insight**: conventional formula-based model can still provide a comparable estimation result to the learning-based one, if its hyperparameters are properly tuned based on hardware.
- Solution: use machine learning to tune the hyper-parameter of the formula-based models.
- Advantage: low cost, generalization, **explainability**



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ParamTree: Learned formula-based cost model

- Two types of parameters:
  - R-params: weight parameter
  - C-params: configuration parameters

HashJoin	startup_cost	cpu	$C_s^L + C_T^R + R_r \times (r_o \times N_{cp} + r_t)$
		disk	$\text{sgn}(nbatches - 1) \times (r_s \times P_r)$
	runtime_cost	cpu	$C_t^L - C_s^L + r_o \times N_{cp} \times R_l + N_{cp} \times r_o \times R_l \times R_r \times innerbucketsize \times 0.5$ $+R_o \times (r_t + r_o \times N_{qp})$
		disk	$\text{sgn}(nbatches - 1) \times (r_s \times (P_r + 2 \times P_l))$

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Objective

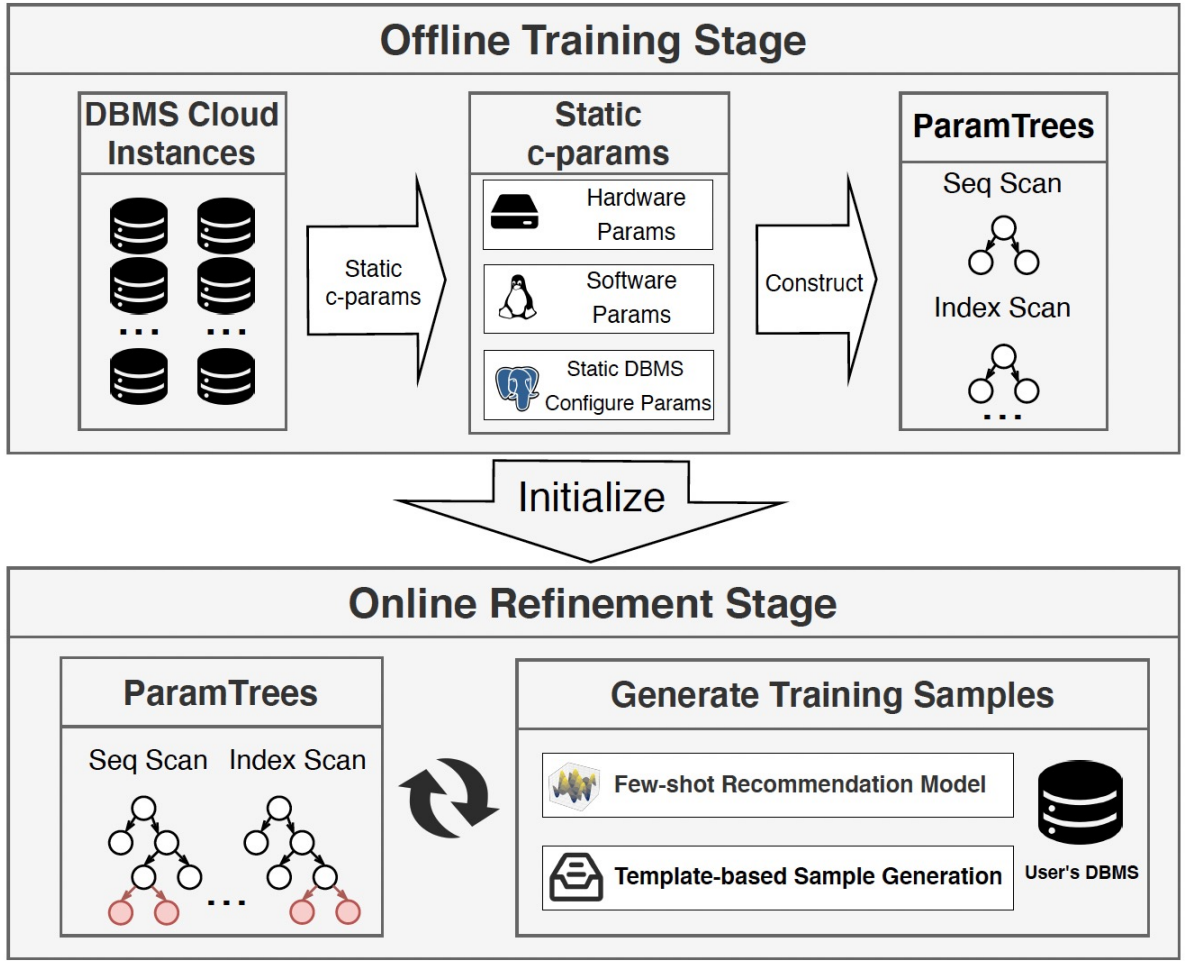
- The objective is to determine optimal choices of R-params in the built-in cost formulas of major databases.
- To accomplish this goal, the paper propose to learn a mapping function from C-params to R-params, to capture their dependencies for a given physical operator *op*.

$$G : C \xrightarrow{\text{op}} R$$

Jiani Yang et al. **Rethinking Learned Cost Models: Why Start from Scratch?** SIGMOD'24

Two-stage training and refinement

- **Offline training stage**: generate an initial decision tree that captures the relationship between R-params and C-params.
- **Online refinement stage**: Online tree expansion is invoked to split the leaf nodes if the **ParamTree** cannot provide a precise estimation for more than λ queries.



Jiani Yang et al. **Rethinking Learned Cost Models: Why Start from Scratch?** SIGMOD'24

ParamTree

- Revisit the three components in ParamTree
- Cardinality estimation: histogram
- Cost estimation: formula-based + learned hyper-parameters
- Plan enumeration: dynamic programming

Summary

- Review the three components in different query optimizers

Component	Traditional query optimizer	Learned Query optimizer	ML-enhanced query optimizer		
			BAO	LERO	ParamTree
Cardinality estimation	Histogram	Tree CNN (implicit)	_	Cardinality as knob	Histogram
Cost estimation	Formula-based	Tree CNN	Tree CNN	Ranking model	Formula-based with learned hyperparameter
Plan enumeration	Dynamic Programming	Value network guided search	Curated Hint set + Expert optimizer	Adjusting cardinality + Expert optimizer	Dynamic Programming

Tutorial Overview

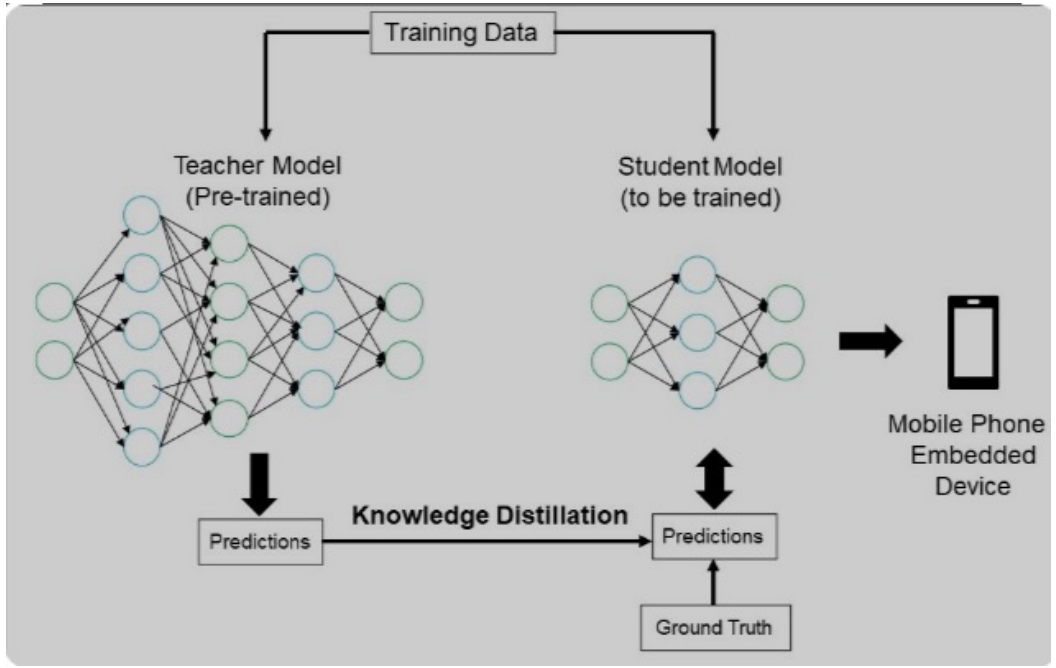
- ML4DB Foundations
- ML4DB Paradigms
- ML4DB Open problems & Opportunities
  1) What are the foundations of ML4DB?
  2) Model efficiency
  3) Generating training data of high quality
  4) Handling data & workload shifts
  5) Foundation models (Pretrained models) for Ml4DB
  6) LLMs for ML4DB

Opportunity 1: What are the foundations of ML4DB?

- Separate ML4DB components are developed. But it might not work to integrate them into DB systems.
- What are the foundations?
  - Query plan representation
  - Pre-trained models
  - Anything else?

Opportunity 2: Model Efficiency

- Ideal model: efficiency in both training & inference
- Potential ML techniques:
  - Light-weight AI models
  - Ad-hoc optimizations
  - Knowledge distillation

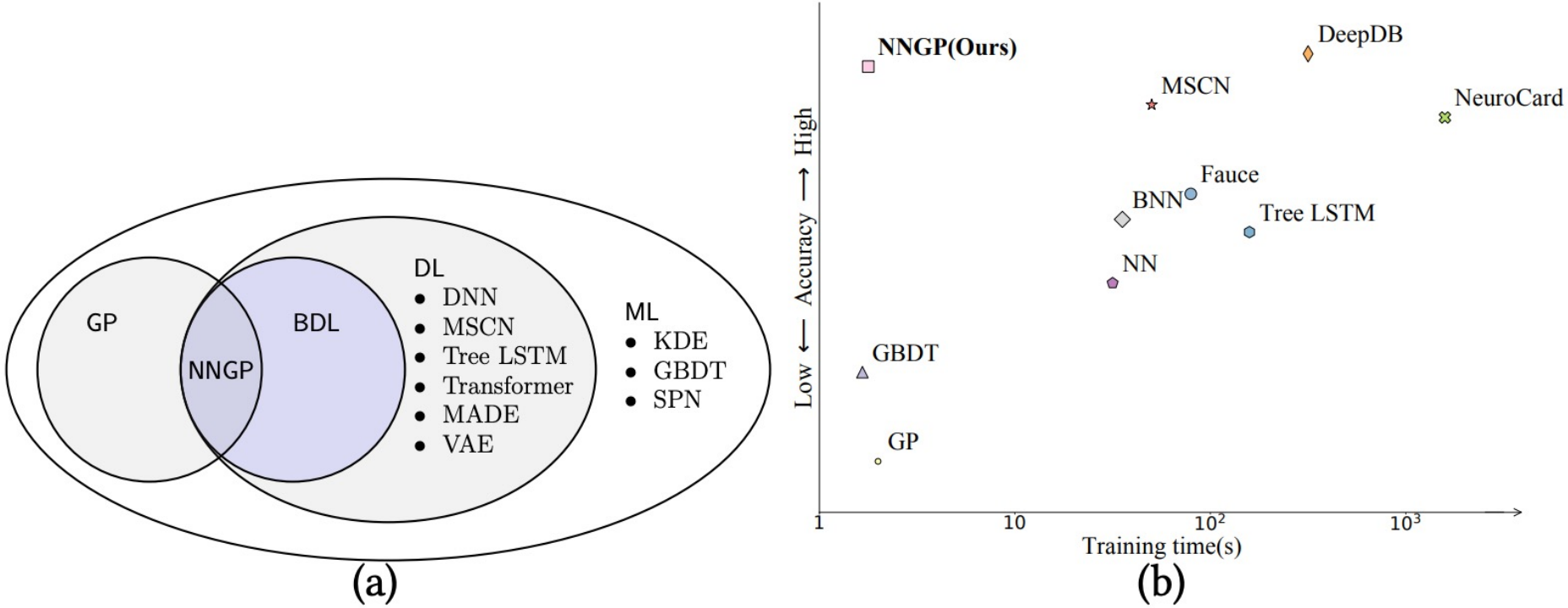


Picture from https://www.analyticsvidhya.com/blog/2022/01/knowledge-distillation-theory-and-end-to-end-case-study/

- Example: Some initial attempts at improving model efficiency for
  - Cardinality estimation
  - Query optimization

Model Efficiency: Cardinality Estimation

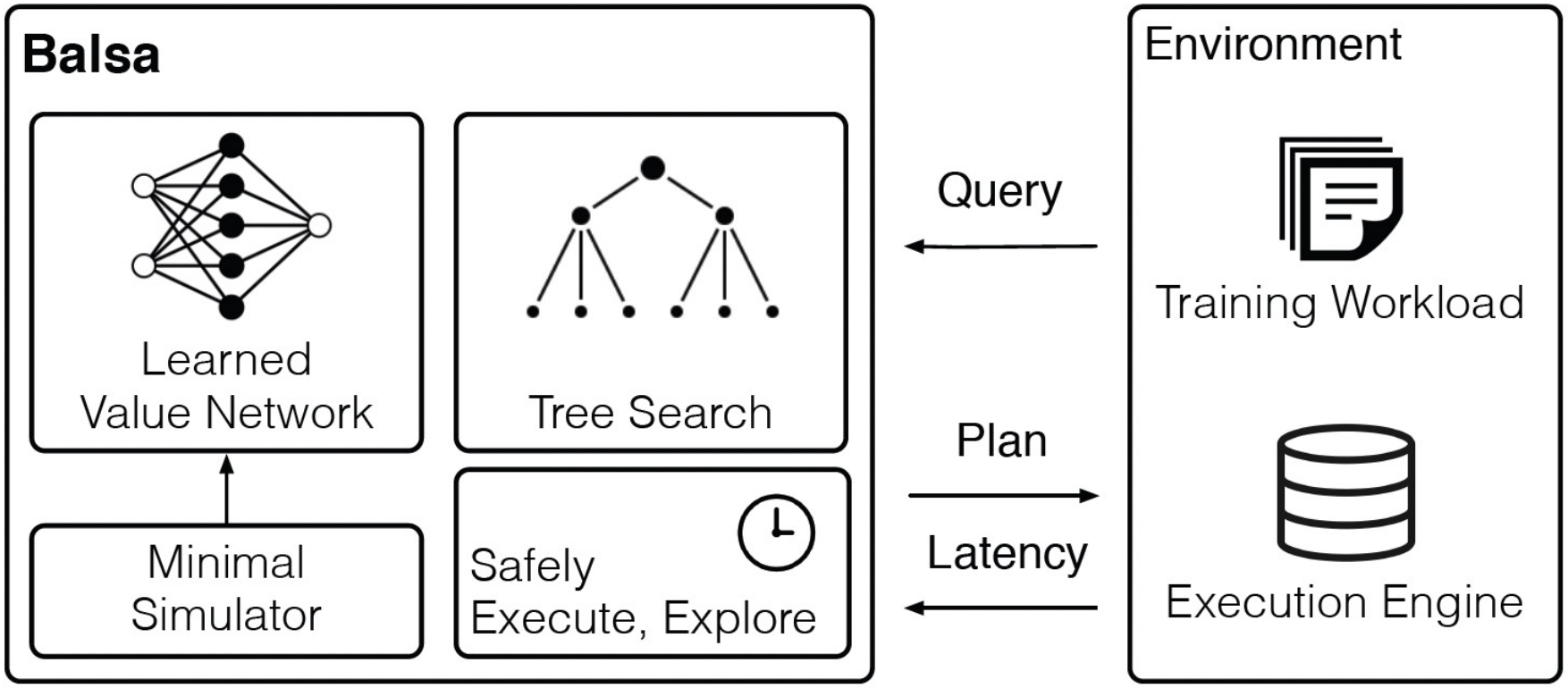
- NNGP (SIGMOD'22): Neural network gaussian process for cardinality estimation



Kangfei Zhao et al. **Lightweight and Accurate Cardinality Estimation by Neural Network Gaussian Process?** SIGMOD'22

Model Efficiency: Query optimization

- Balsa (SIGMOD'22): Simulation-to-reality learning and safe execution



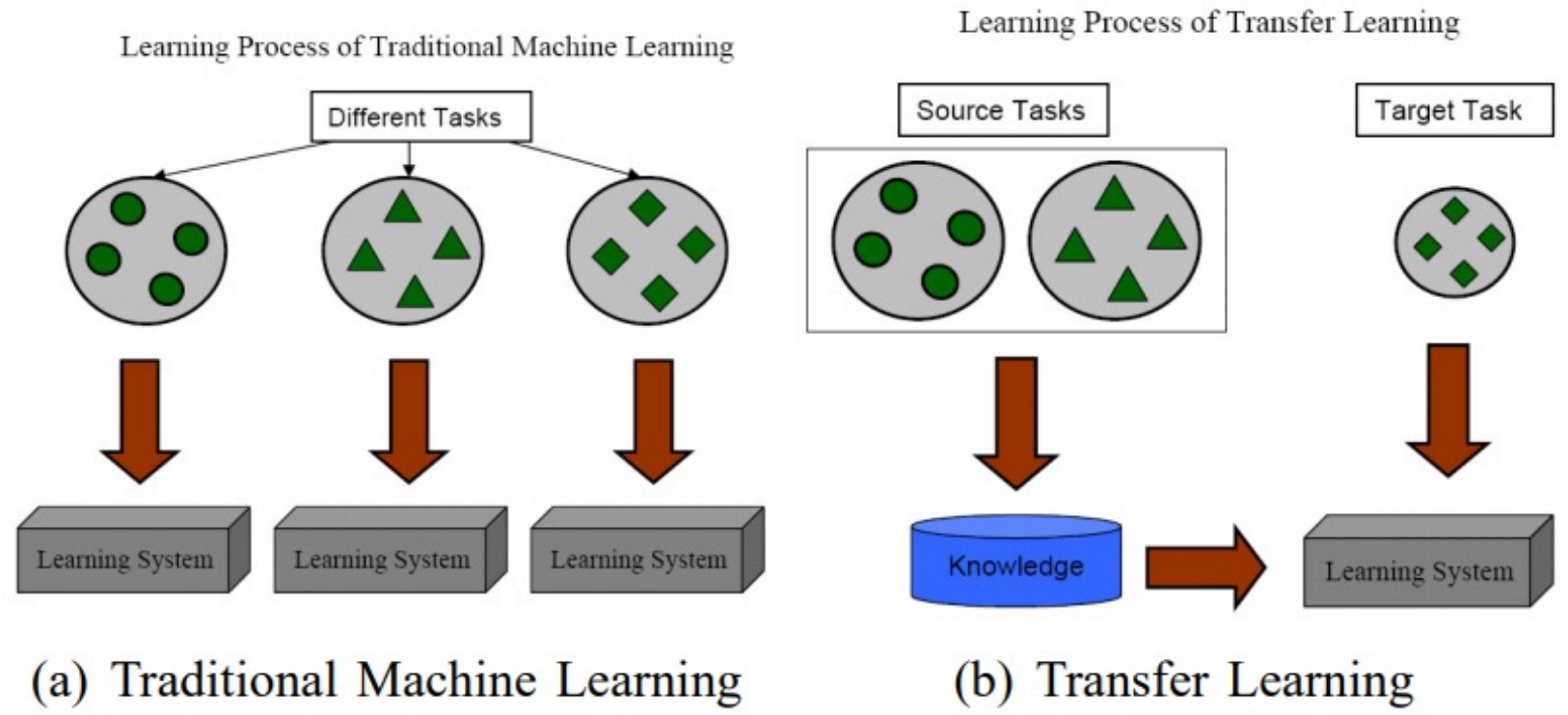
Yang et al. **Balsa: Learning a Query Optimizer Without Expert Demonstrations** SIGMOD'22

Opportunity 3: Handling data & workload shifts

- Most machine learning models require retraining in face of data & workload shifts, which can be very costly.
- Potential ML techniques
  - Transfer learning
  - Meta-learning
  - Domain generalization and adaptation
- Some models that adapt to data & workload shift
  - Cardinality estimation (Beibin Li et al., SIGMOD'22; Parimarjan Negi et al., SIGMOD'23; Zilong Wang et al., VLDB'23)
  - Data generation

Transfer Learning

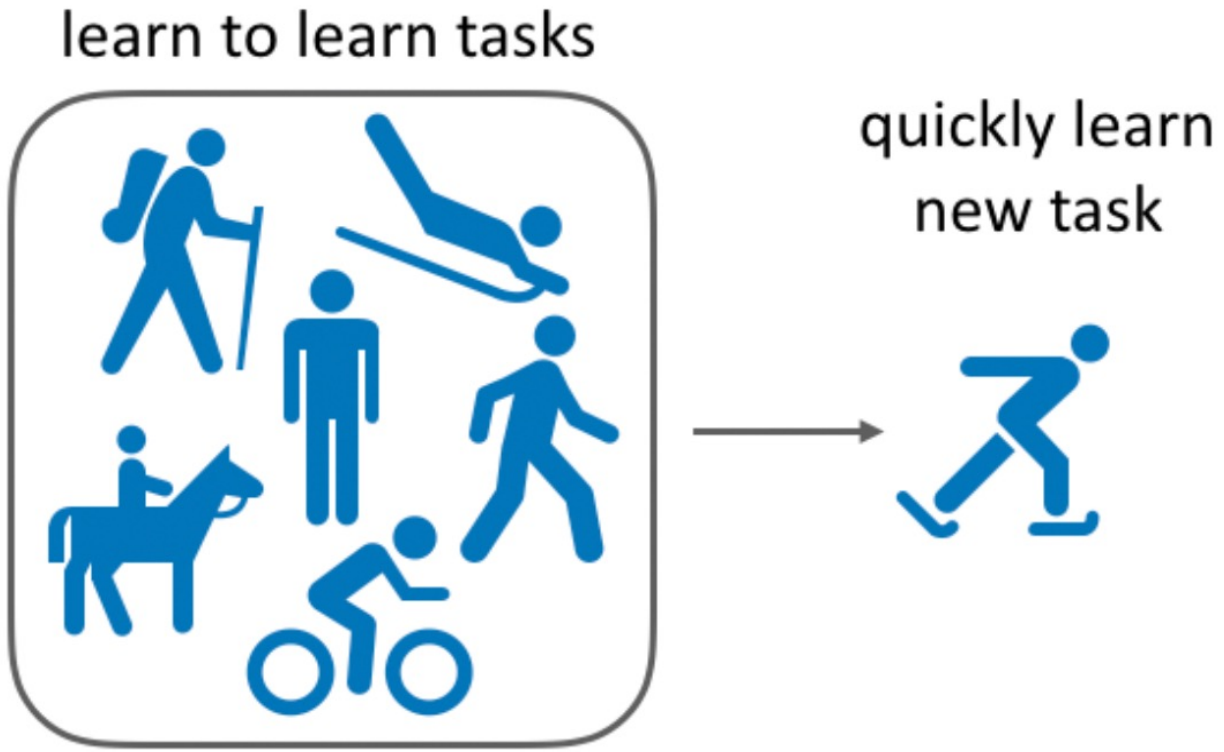
- Improve the target learners on target domains by transferring the knowledge contained in different but related source domains.



Pictures from Hosna, A et al, Transfer learning: a friendly introduction. Journal of Big Data (2022)

Meta-learning

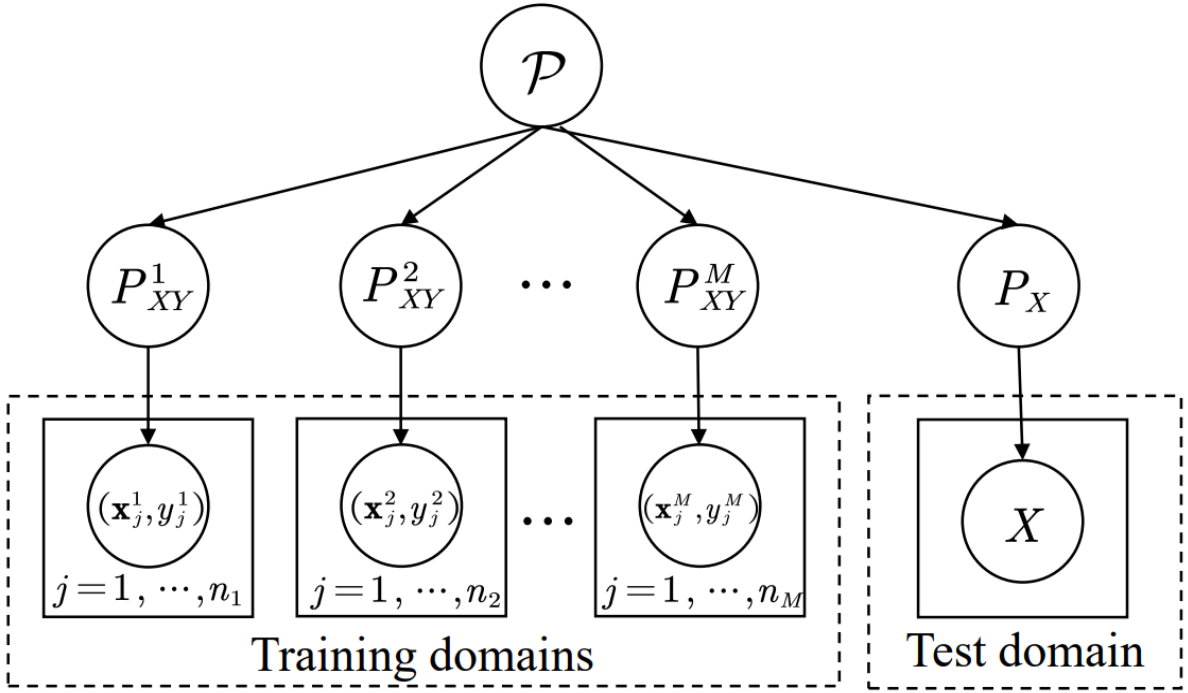
- Meta-learning aims to learn the learning algorithm itself by learning from previous experience or tasks, i.e., learning-to-learn.



Pictures from Huisman, Mike, Jan N. Van Rijn, and Aske Plaat. "A survey of deep meta-learning." Artificial Intelligence Review 54.6 (2021): 4483-4541.

Domain generalization

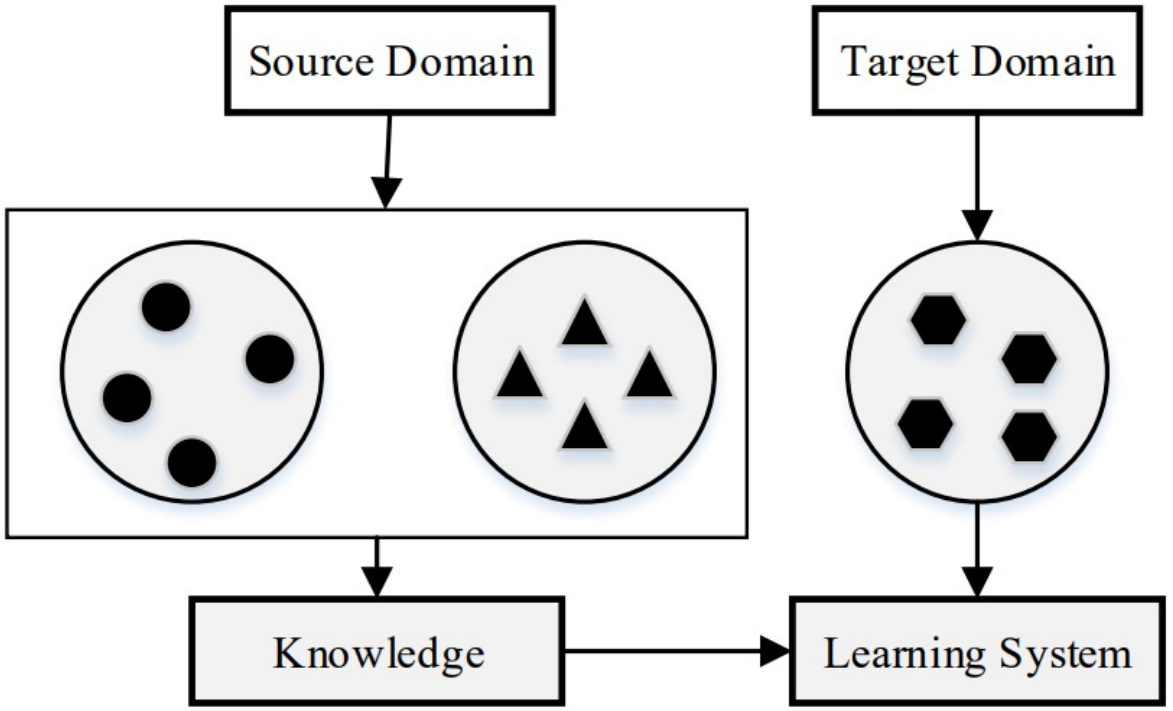
- Domain generalization leverage common knowledge learned from multiple training domains to generalize to unseen test domains.



Pictures from Wang, Jindong, et al. "Generalizing to unseen domains: A survey on domain generalization." TKDE 35.8 (2022): 8052-8072

Domain adaptation

- Domain adaptation aims to maximize the performance on a given target domain using existing training source domain(s).



Pictures from Wang, Mei, and Weihong Deng. "Deep visual domain adaptation: A survey." Neurocomputing 312 (2018): 135-153

Handling data & workload shifts: cardinality estimation

- Warper (SIGMOD'22): generate additional queries when limited examples are available and pick the queries to update the model

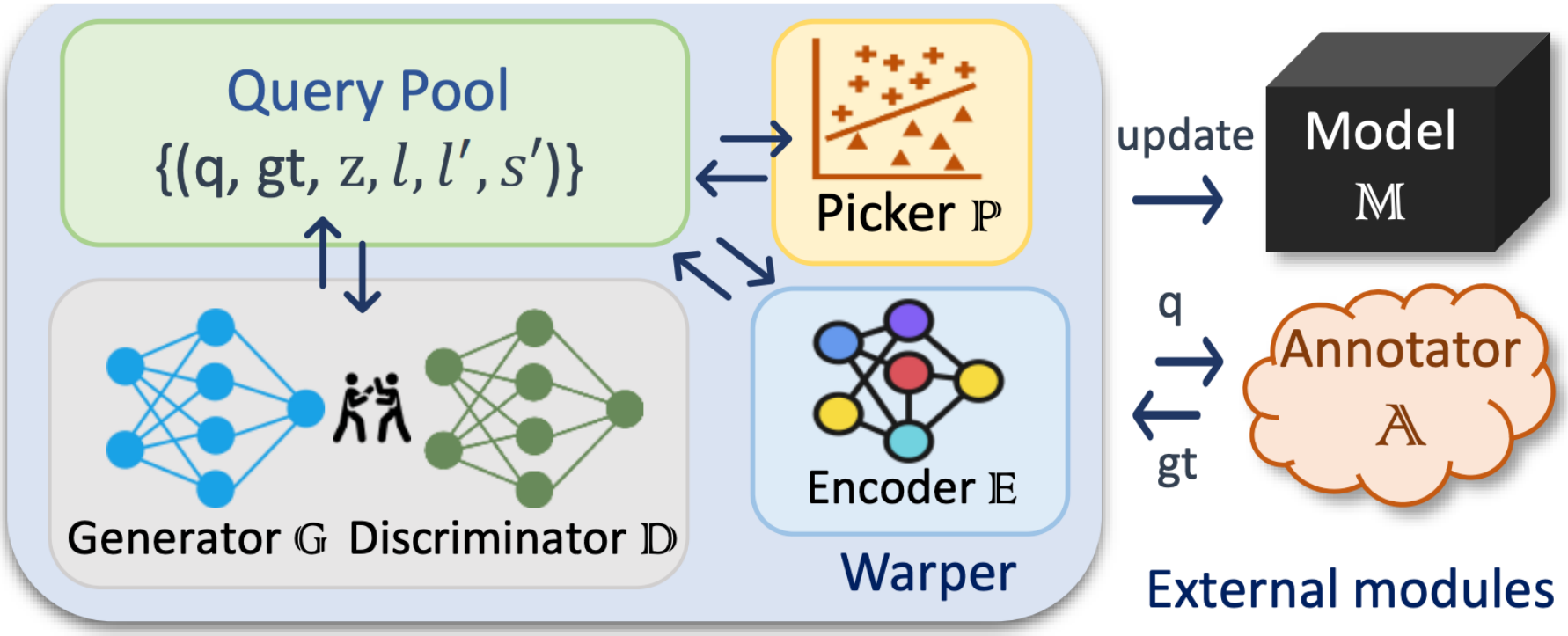


Figure from Beibin Li et al., **Warper: Efficiently adapting learned cardinality estimators to data and workload drifts.** SIGMOD'22

Handling data & workload shifts: data generation

- DDUp (SIGMOD'23): Statistical test for detecting data shifts, and incrementally update the model through knowledge distillation

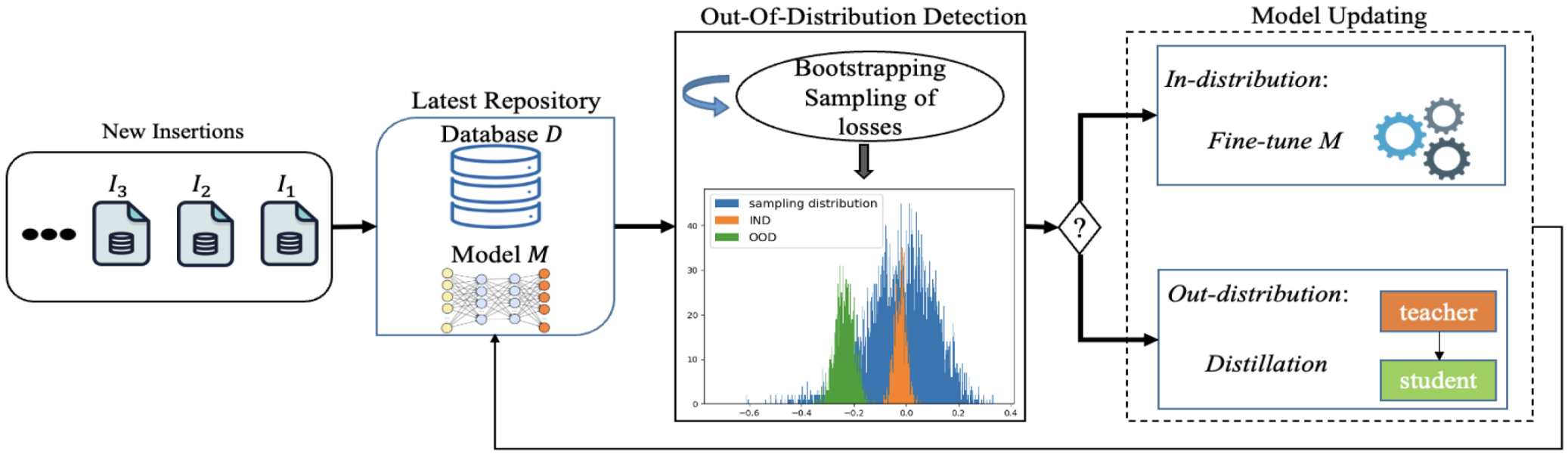


Figure from Meghdad Kurmanji et al., **Detect, Distill and Update: Learned DB Systems Facing Out of Distribution Data.** SIGMOD'23

Opportunity 4: Training data of high quality

We want to generate both datasets and query workload. Ideally,

1. Diverse Workloads
   - Include a variety of queries, from simple SELECT statements to complex operations.
2. Comprehensive Coverage
   - Include data from various domains (e.g., finance, healthcare, e-commerce) with different underlying distribution.
3. Annotated with Performance Metrics
   - Include detailed performance metrics such as query execution times, resource usage, throughputs, etc.
   - Annotate data with configuration settings and their impact on performance.

   ….

- But, even for a single ML4DB task, training data are generated by executing queries on a DBMS to collect the physical plan and corresponding cost. Very expensive !!!

Opportunity 5: Foundation (Pretrained) models for ML4DB tasks

- ML4DB models are typically trained on a specific database with specific hardware/software configuration
- Retraining is required when transferring to a new database or different hardware/software environment or a new task
- Can we have a large pretrained model for ML4DB?
  - Capability to generalize to different data
  - Capability to generalize across tasks
  - Capability to generalize across hardware/software

Opportunity 5: Foundation (Pretrained) models for ML4DB tasks

- Challenges
  - Lack of large collection of **databases and query workload, and training data**
  - Designing **scalable** pre-training methods
  - Identifying and integrating the most relevant **features**
  - Designing models that support **incremental** learning
  - **Integrating** pre-trained models with current database management systems
- Some pioneering attempts
  - Hilprechet & Binnig CIDR21, VLDB22
  - Paul et al VLDB22,
  - Wu et al, CIDR22

Opportunity 6: LLMs for ML4DB tasks

- What can LLMs do for DBs?
- Some pioneering attempts
  - Text2SQL (Many works)
  - Database tunning [1, 2]
  - DBA [3]
  - Query rewriting [4]
  - Interaction with data systems [5]
  - ...

Huang, X et al, LLMTune: Accelerate Database Knob Tuning with Large Language Models. arXiv 2024. [1]
Lao, J et al. GPTuner: A Manual-Reading Database Tuning System via GPT-Guided Bayesian Optimization. VLDB 2024. [2]
Zhou, X et al. LLM As DBA. arXiv 2023. [3]
Li, Z et al. LLM-R2: A Large Language Model Enhanced Rule-based Rewrite System for Boosting Query Efficiency. arXiv 2024 [4]
Xue, S et al. Demonstration of DB-GPT: Next Generation Data Interaction System Empowered by Large Language Models. arXiv 2024. [5]

THANK YOU!

The slides will be made available on our group website