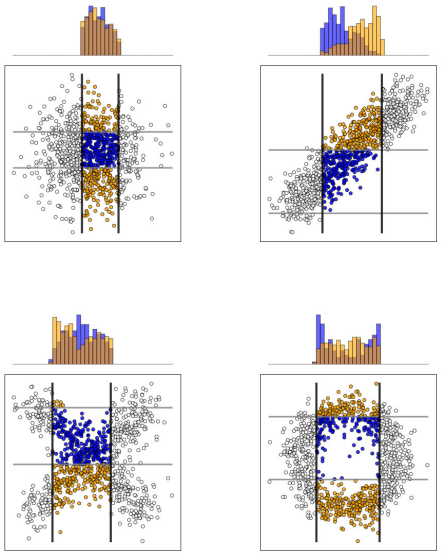
Karlsruhe Institute of Technology

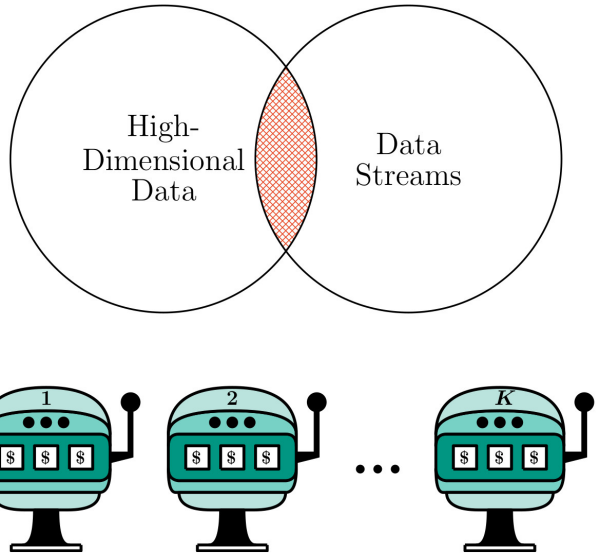
Estimating Dependency, Monitoring and Knowledge Discovery in High-Dimensional Data Streams

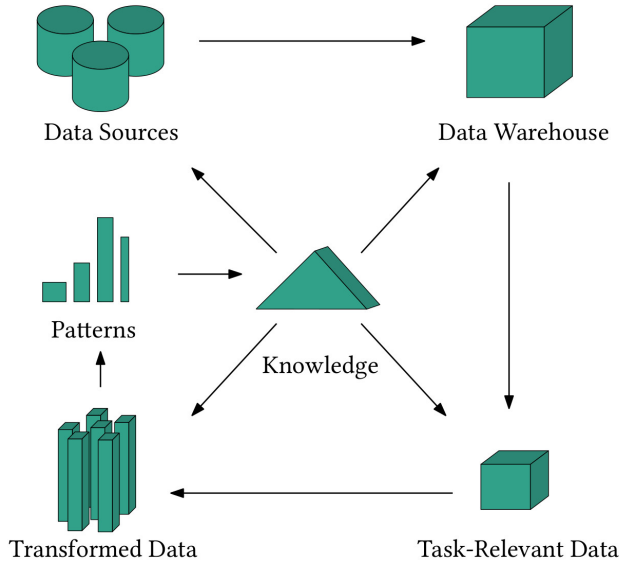
Doctoral Defense

Edouard Fouché | July 15, 2020

ADVISOR: PROF. DR.-ING. KLEMENS BÖHM







Motivations

Data Mining – or *Knowledge Discovery from Data (KDD)* – is the process of extracting knowledge from massive data sets.

- Data Mining has massive impact on our daily lives.

Modern tasks often involve data that:

- is *high-dimensional* (many attributes)
- comes as a *stream* (continuously collected)
- or both ! (high-dimensional + stream)

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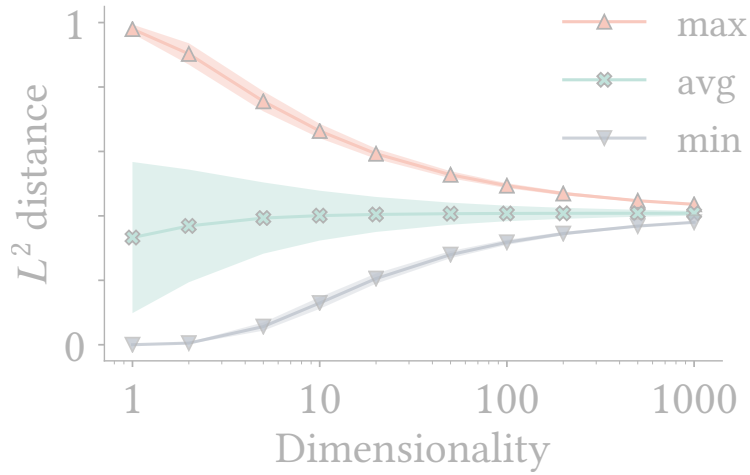
Challenges

We must deal with *High-Dimensional Data Streams (HD-DS)*.
→ They come with two sets of challenges:

High-Dimensionality

"*curse of dimensionality*" [Bel57]

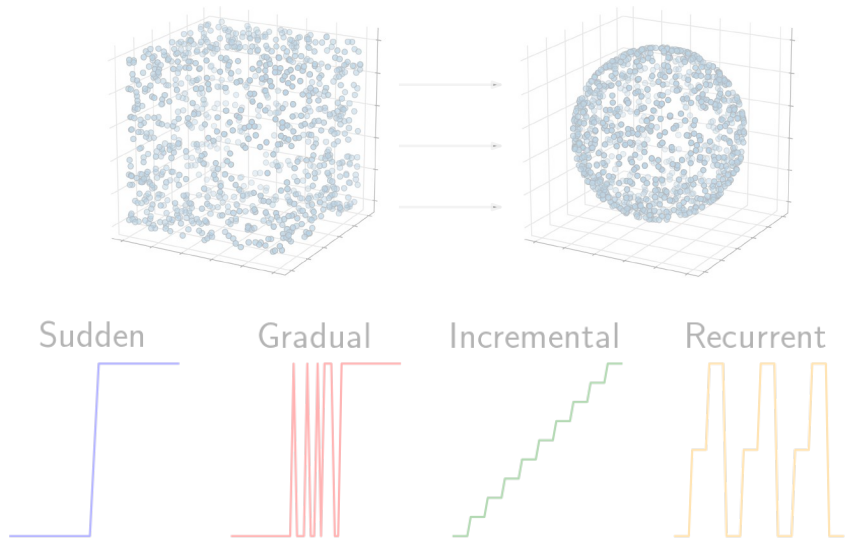
- The space becomes sparse
- Number of subspaces ↗
- *Robust*/*efficient* algorithms



Data Streams

"*concept drift*" [BGE15]

- Data may change over time
- *Adaptive* techniques



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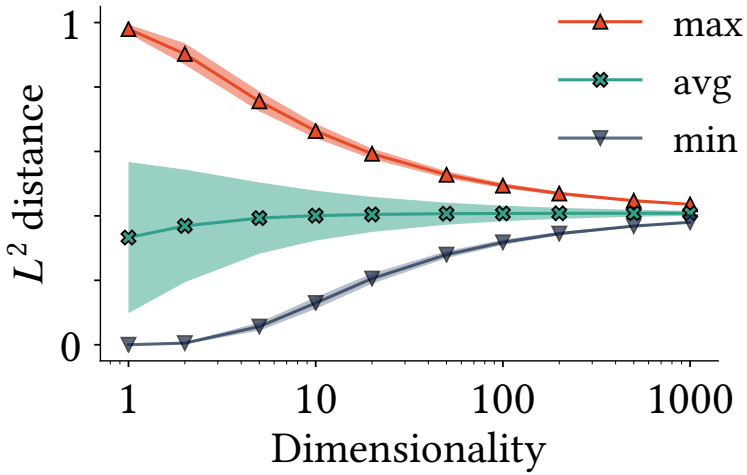

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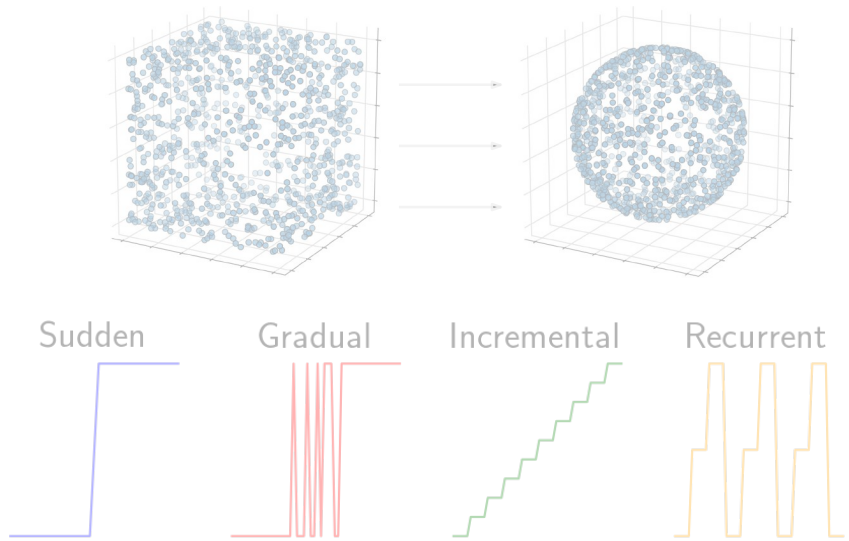

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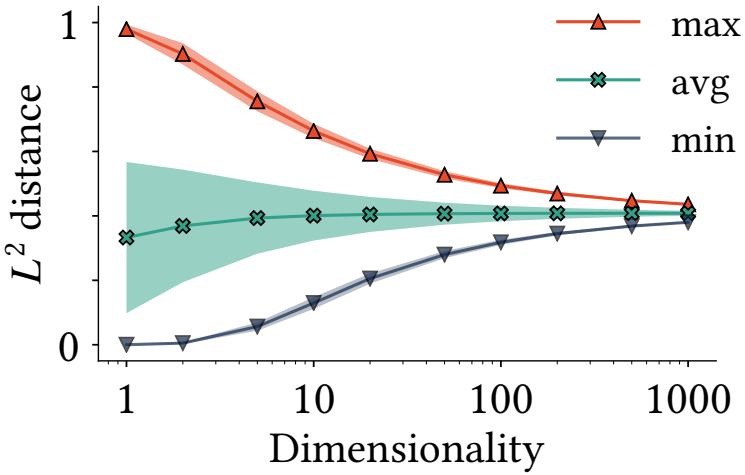

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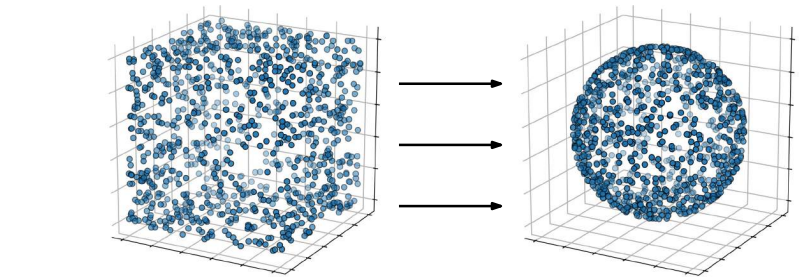

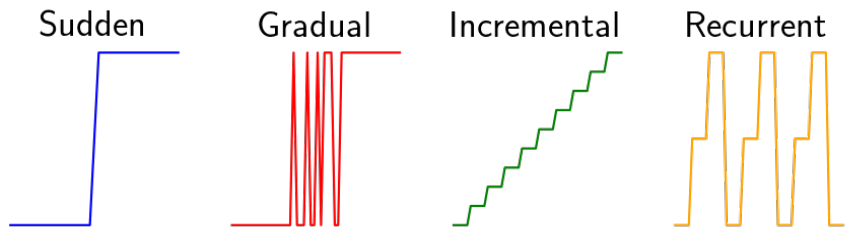

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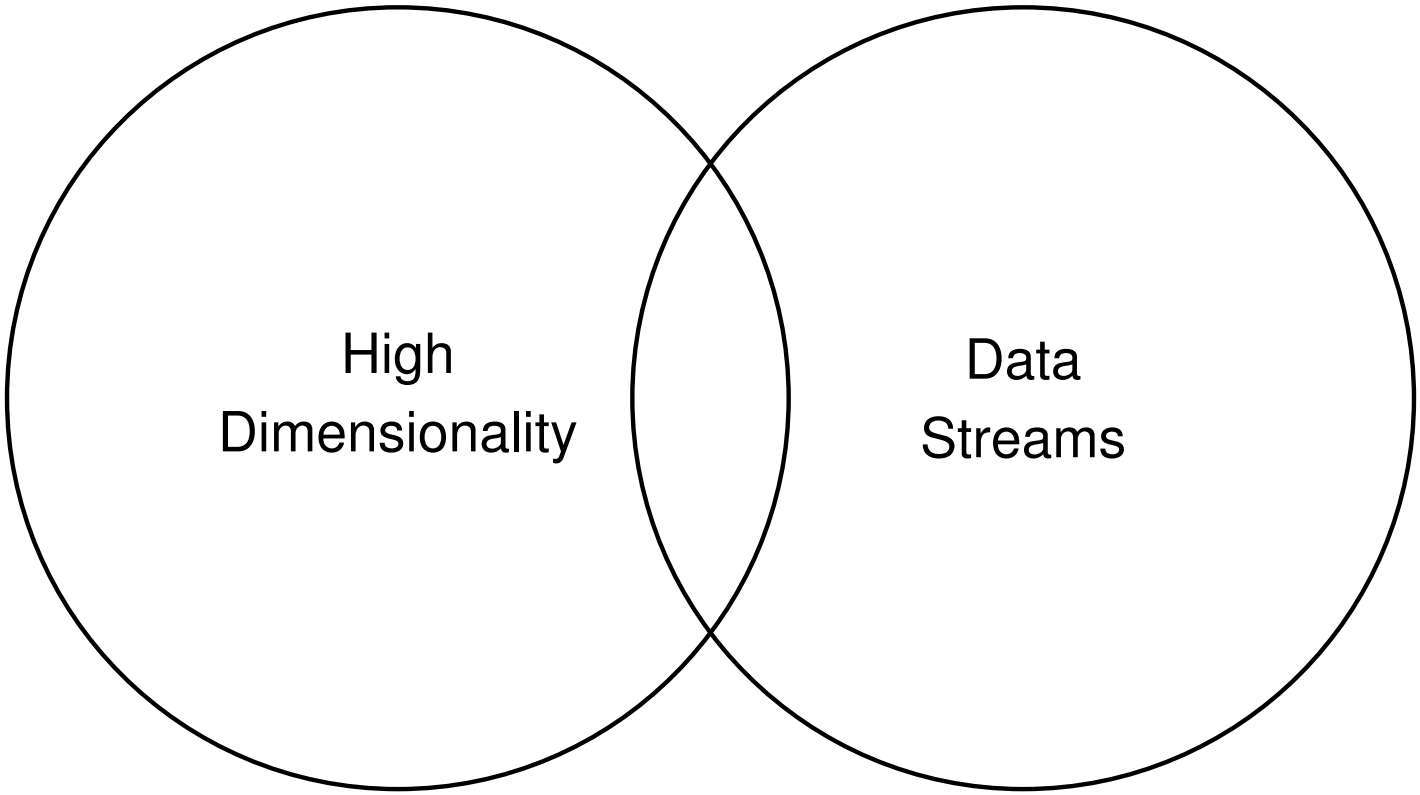

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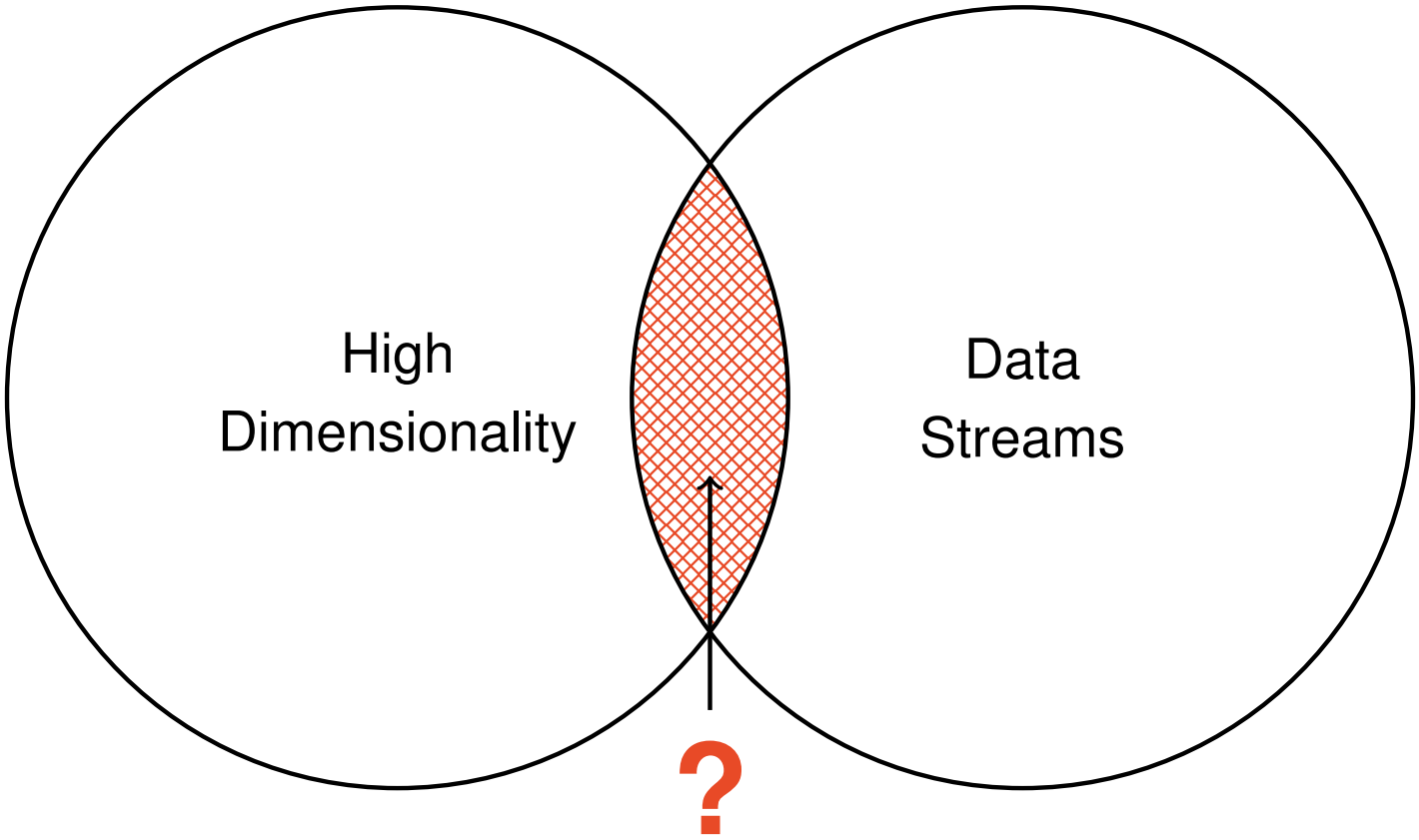

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The Role of Dependency Estimation

- Dependency/Correlation:
  - Describes the strength of relationship between attributes
  - In practice: Can only be estimated from empirical observations
  - Examples: Pearson, Spearman, Mutual Information (MI), ...
- Plays a central role in the KDD process

→ An open problem with *High-Dimensional Data Streams* !

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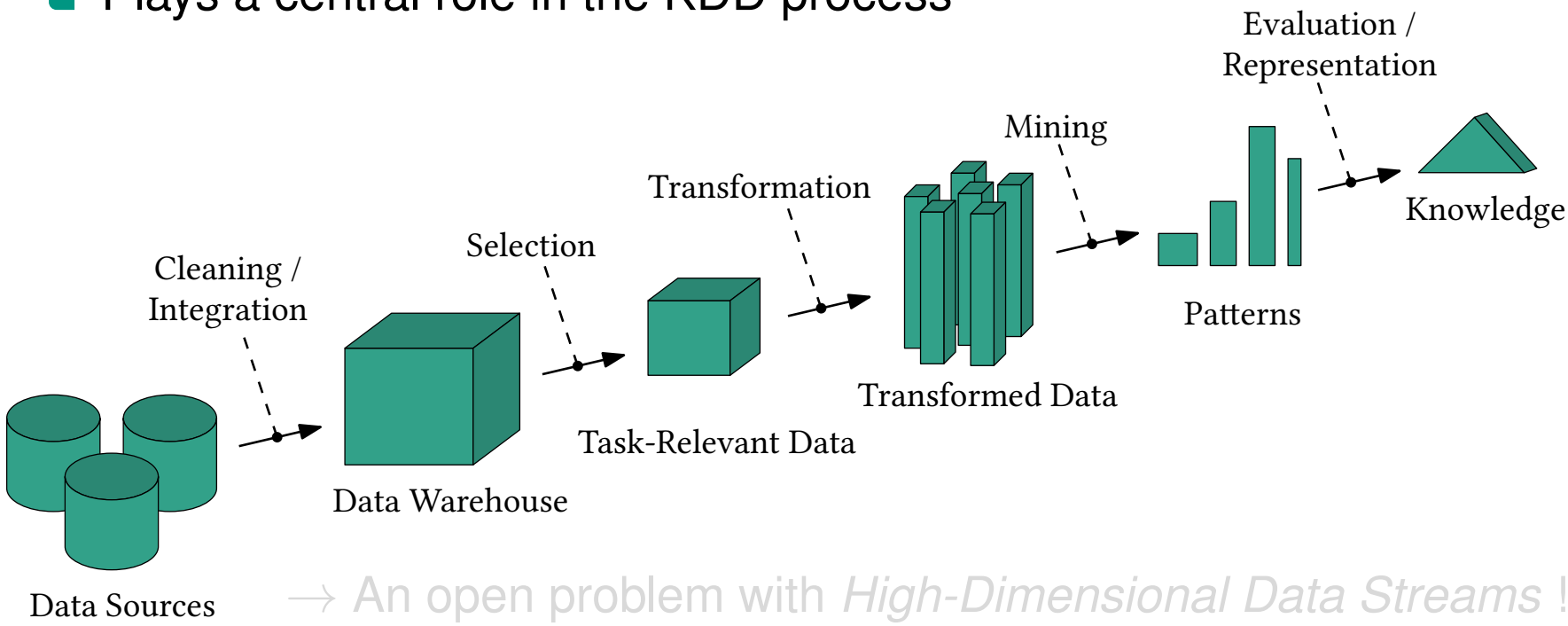

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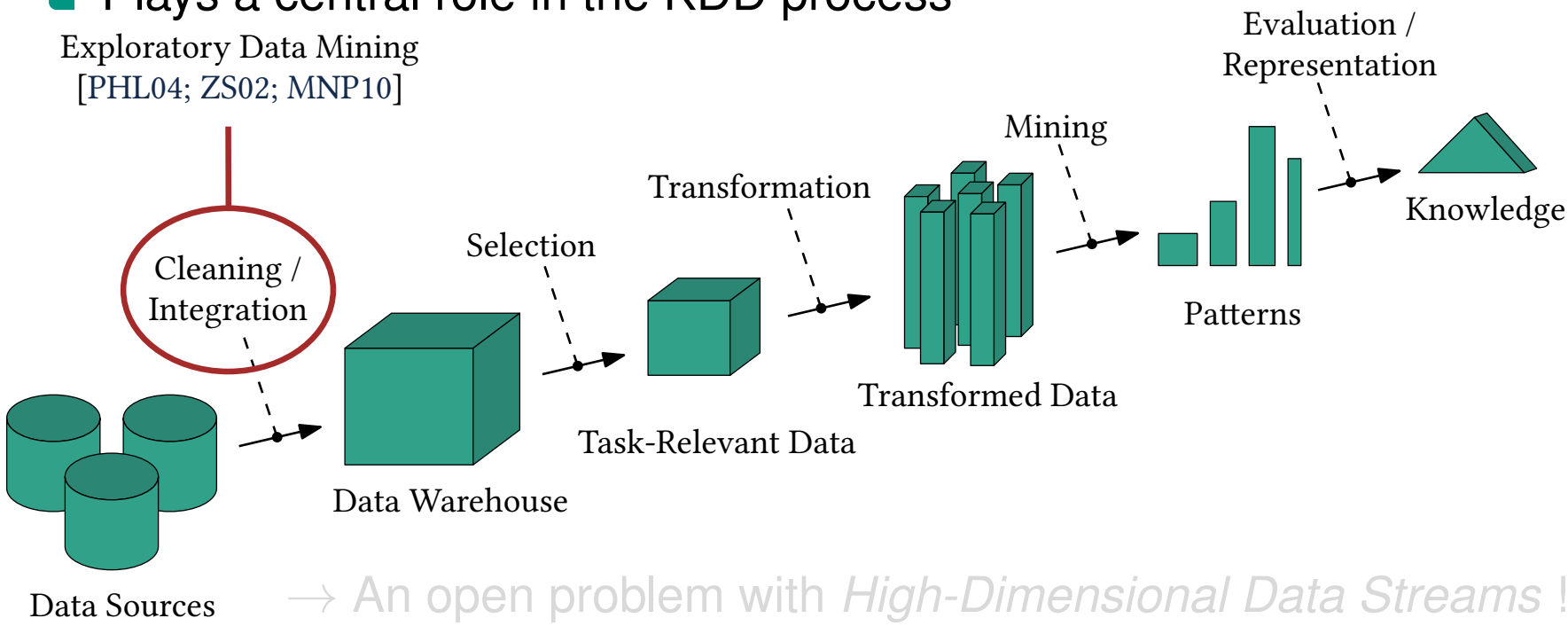

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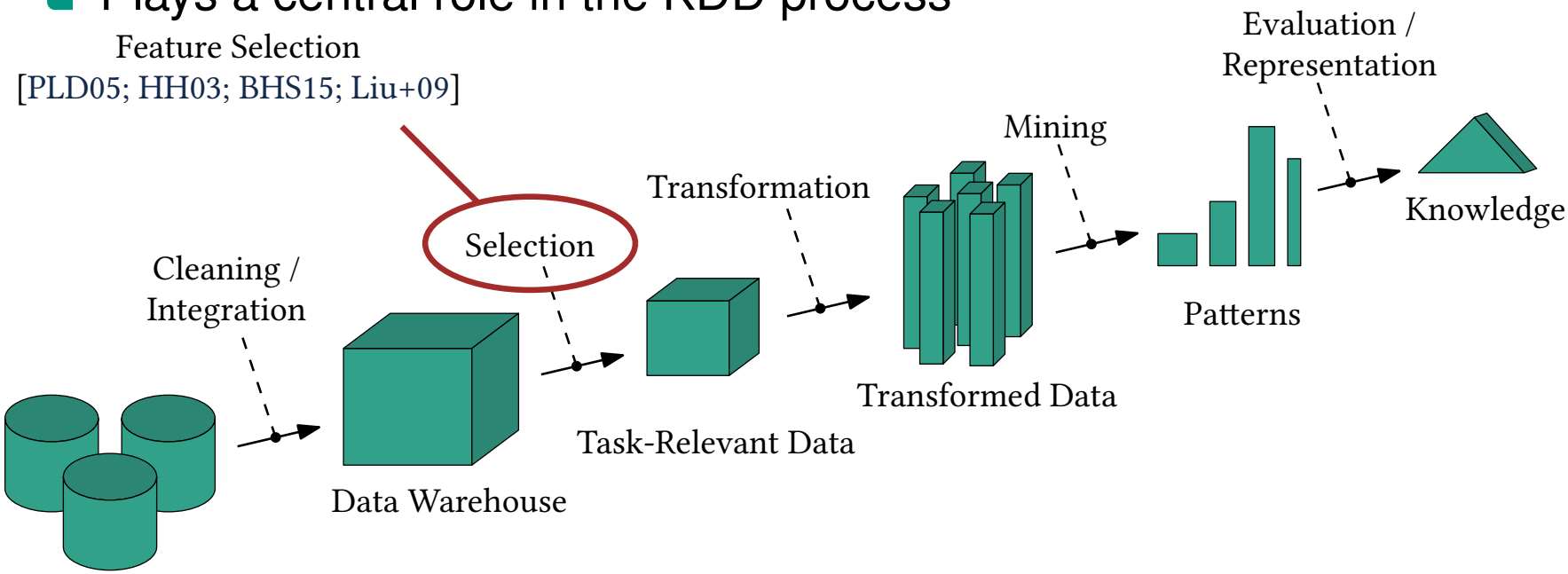

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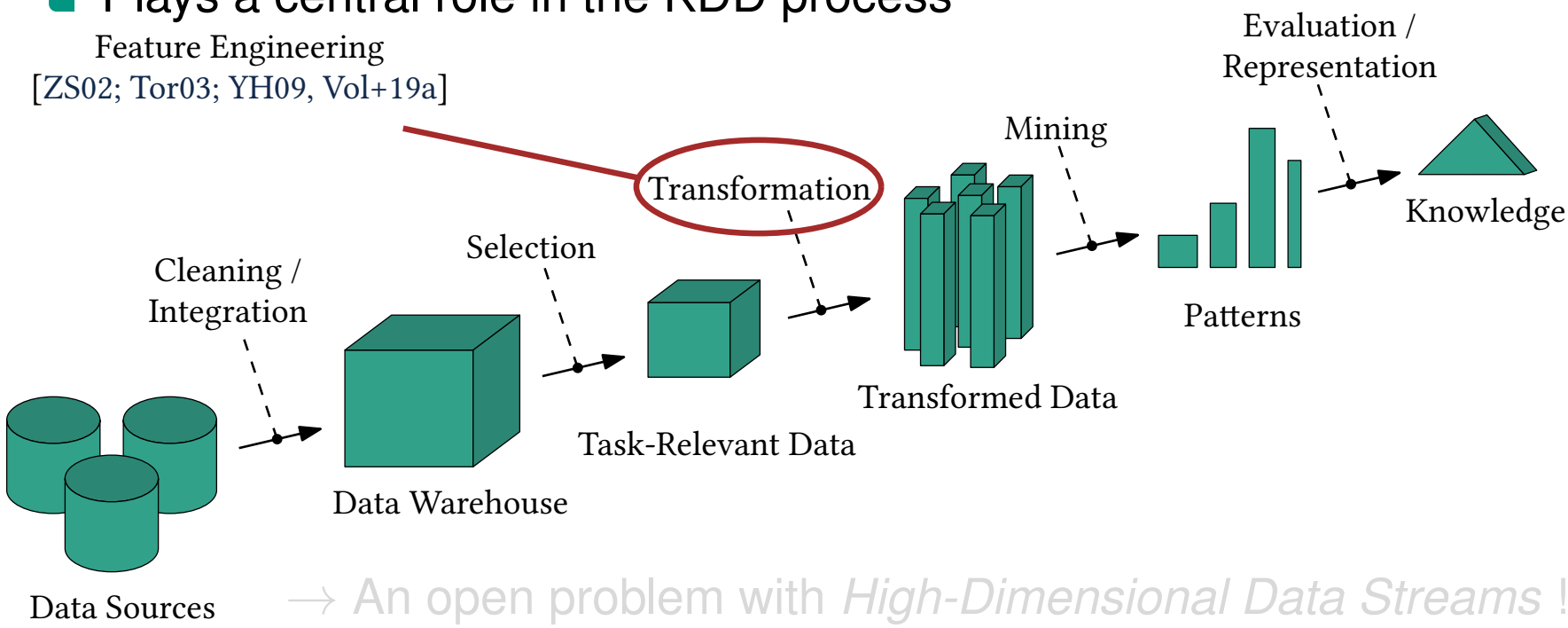

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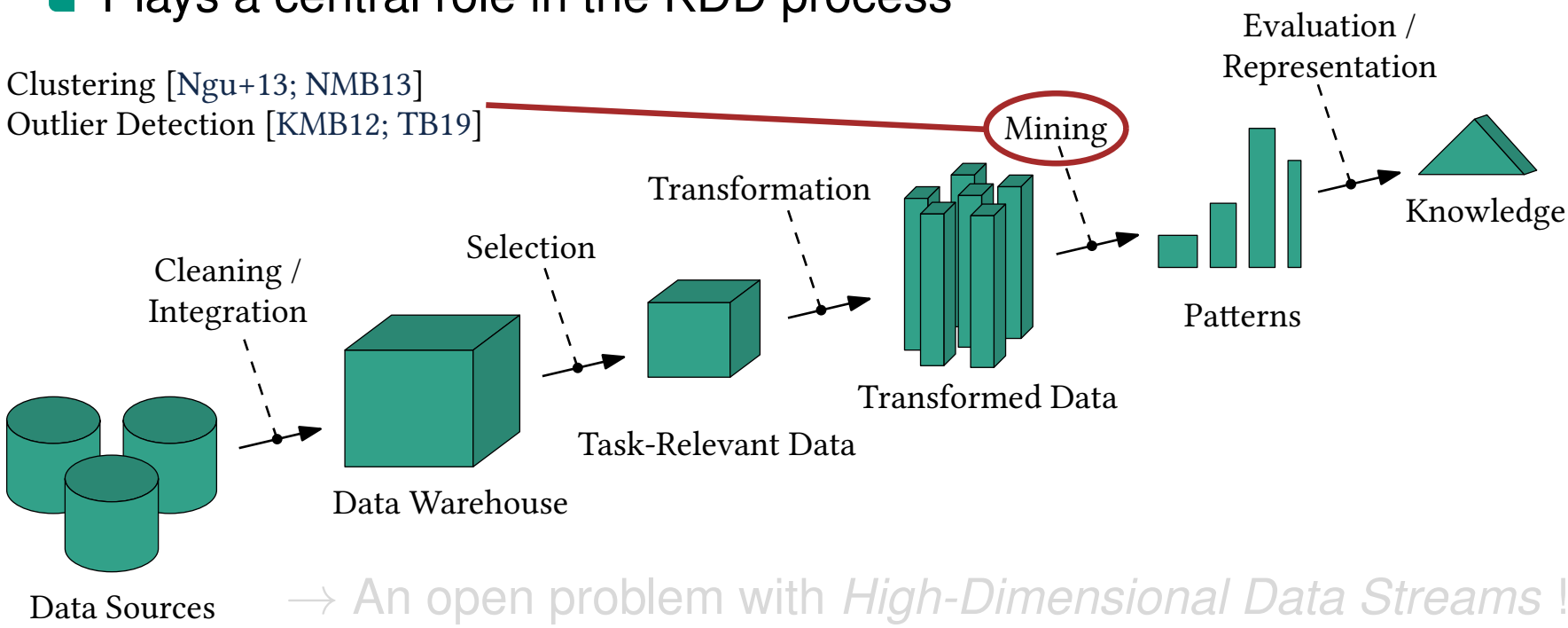

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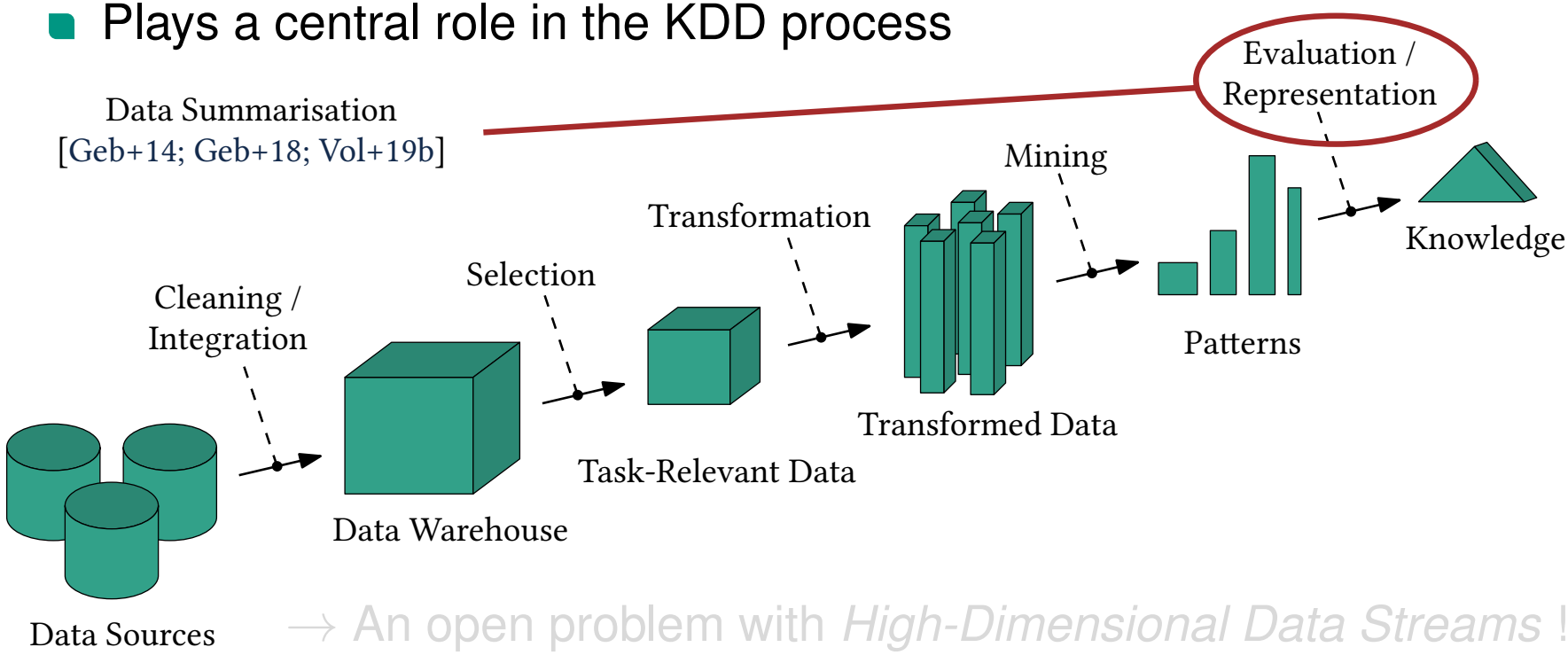

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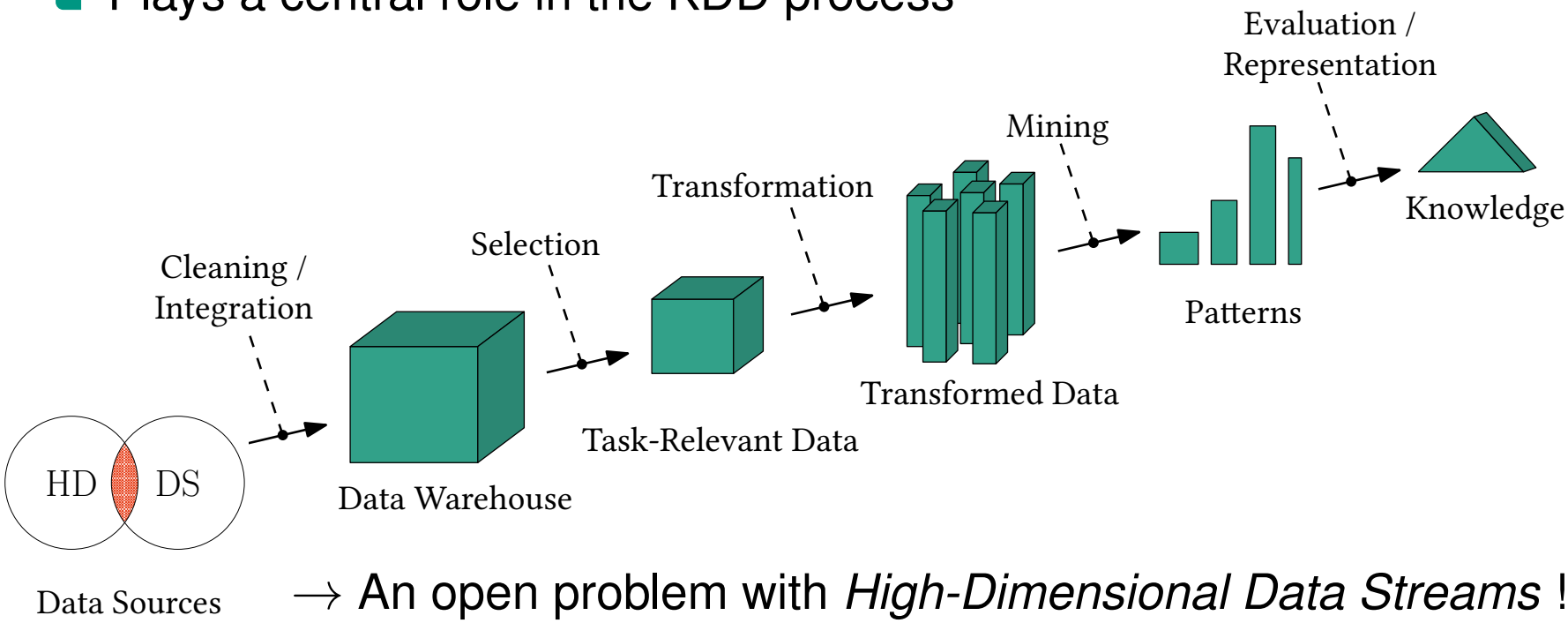

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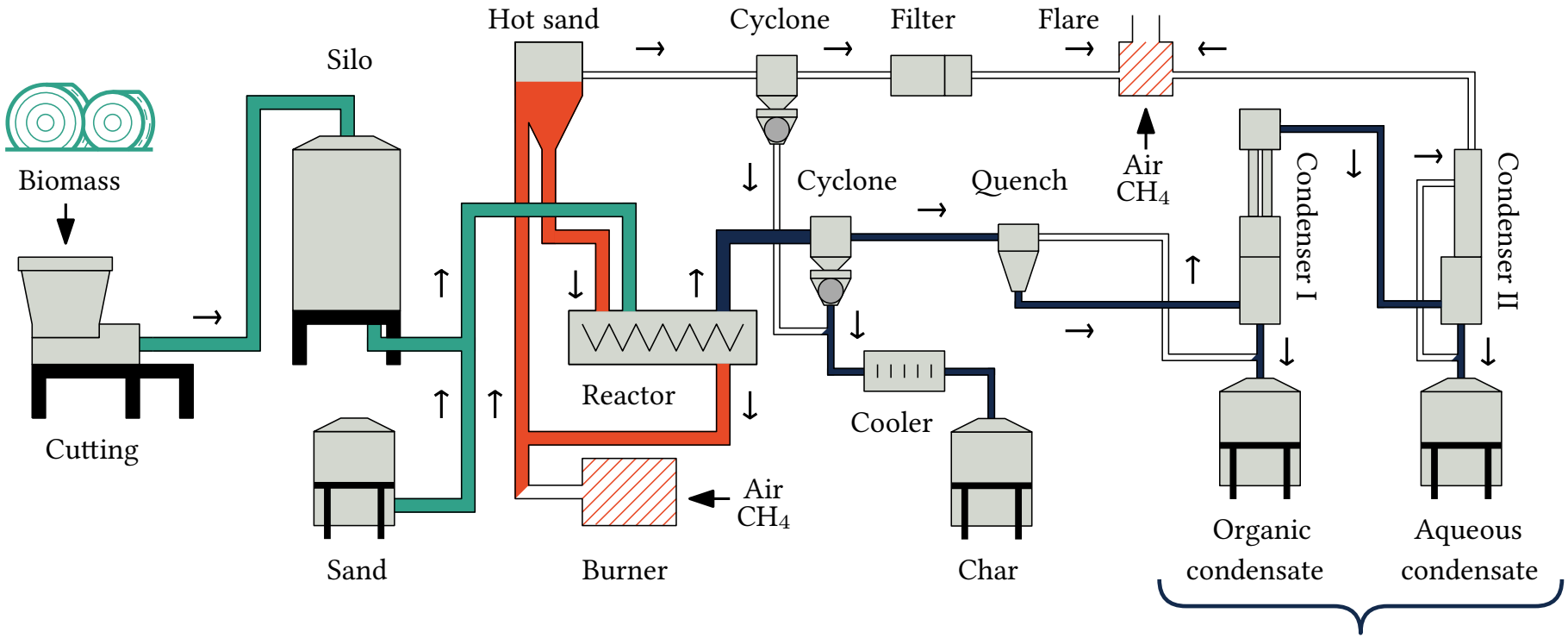
Bioliq®: The pyrolysis as a HD-DS



Simplified schematics of Bioliq's Pyrolysis

- $>$ 400 sensors, continuously measured $\rightarrow$ HD-DS
- Data Mining may help to analyse the pyrolysis process

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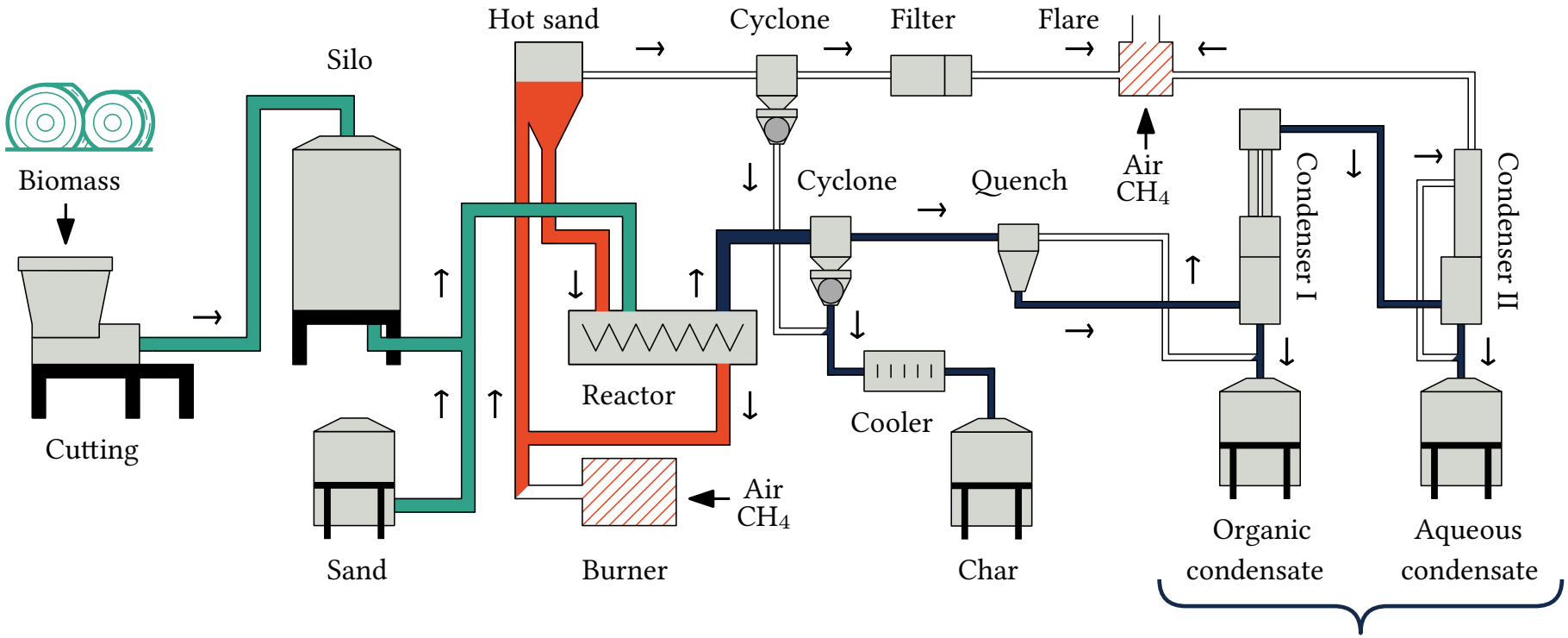

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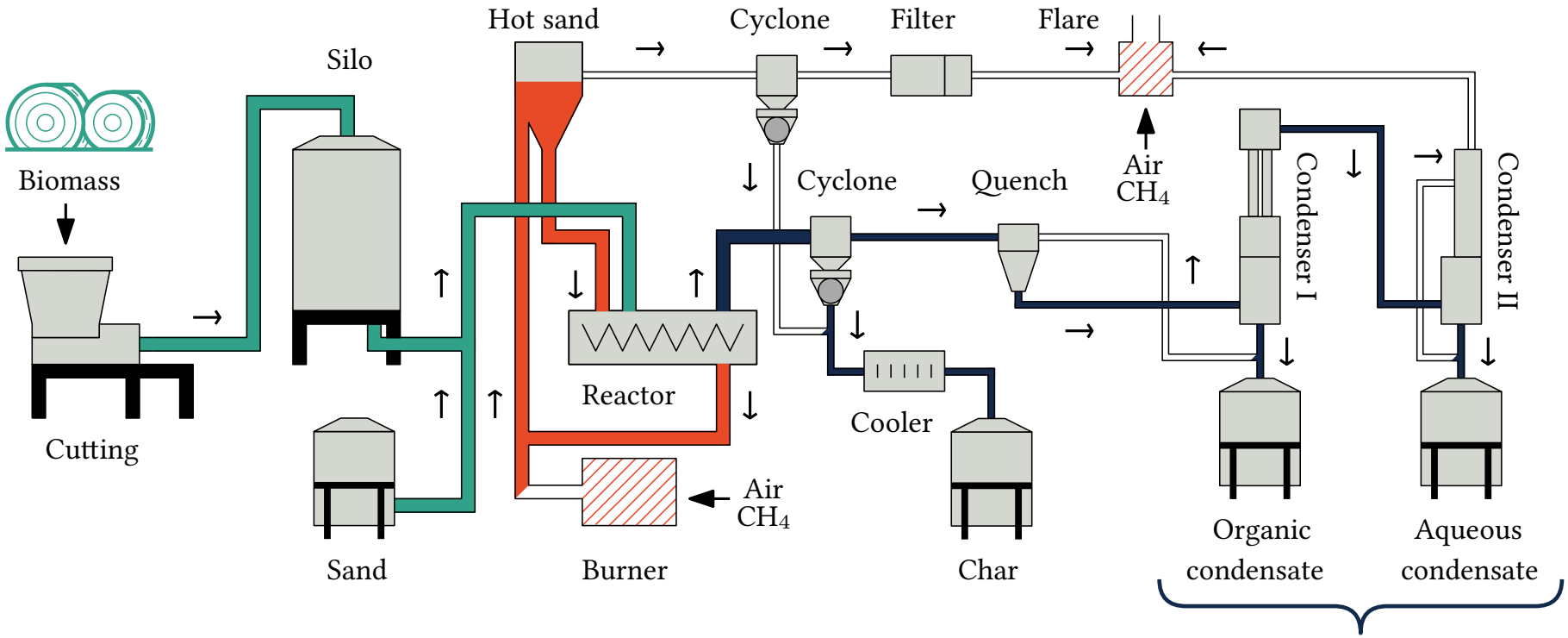

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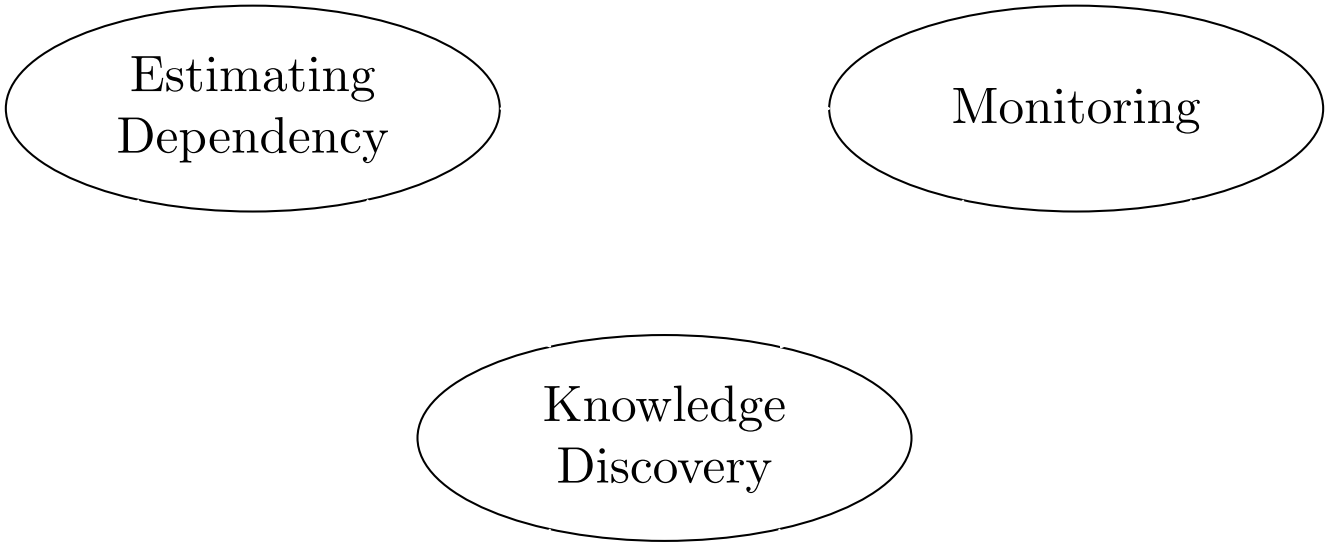

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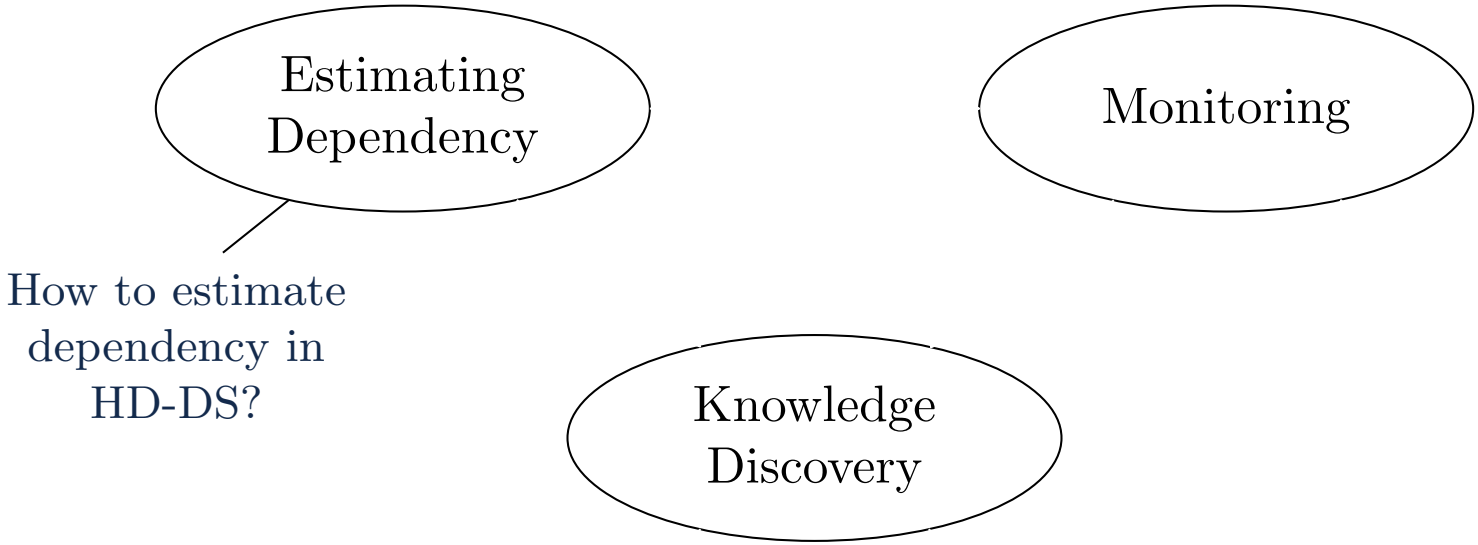

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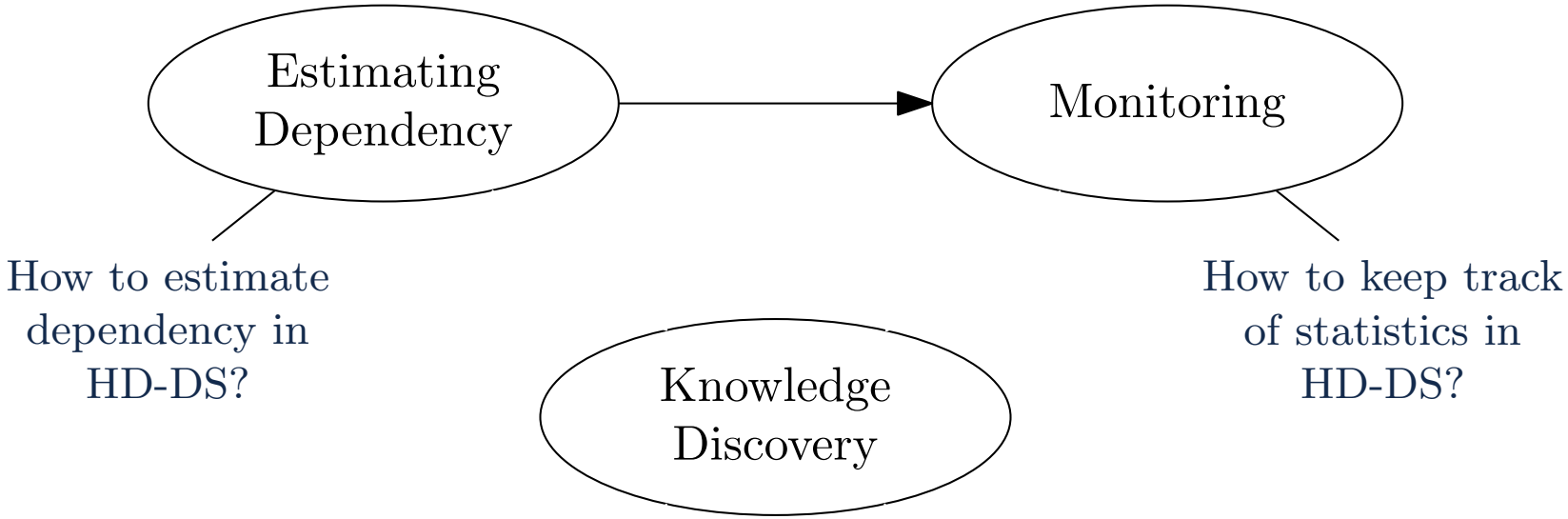

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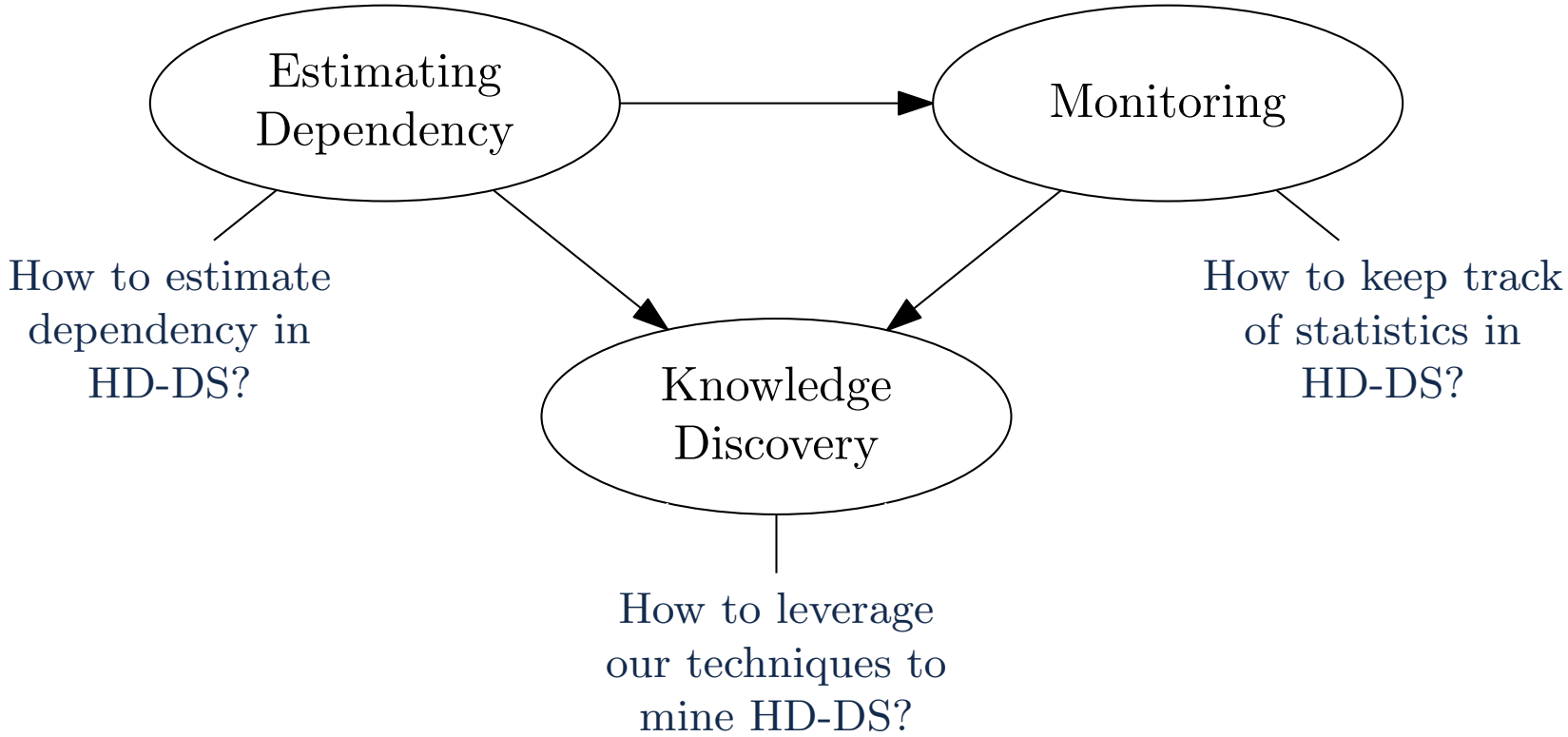

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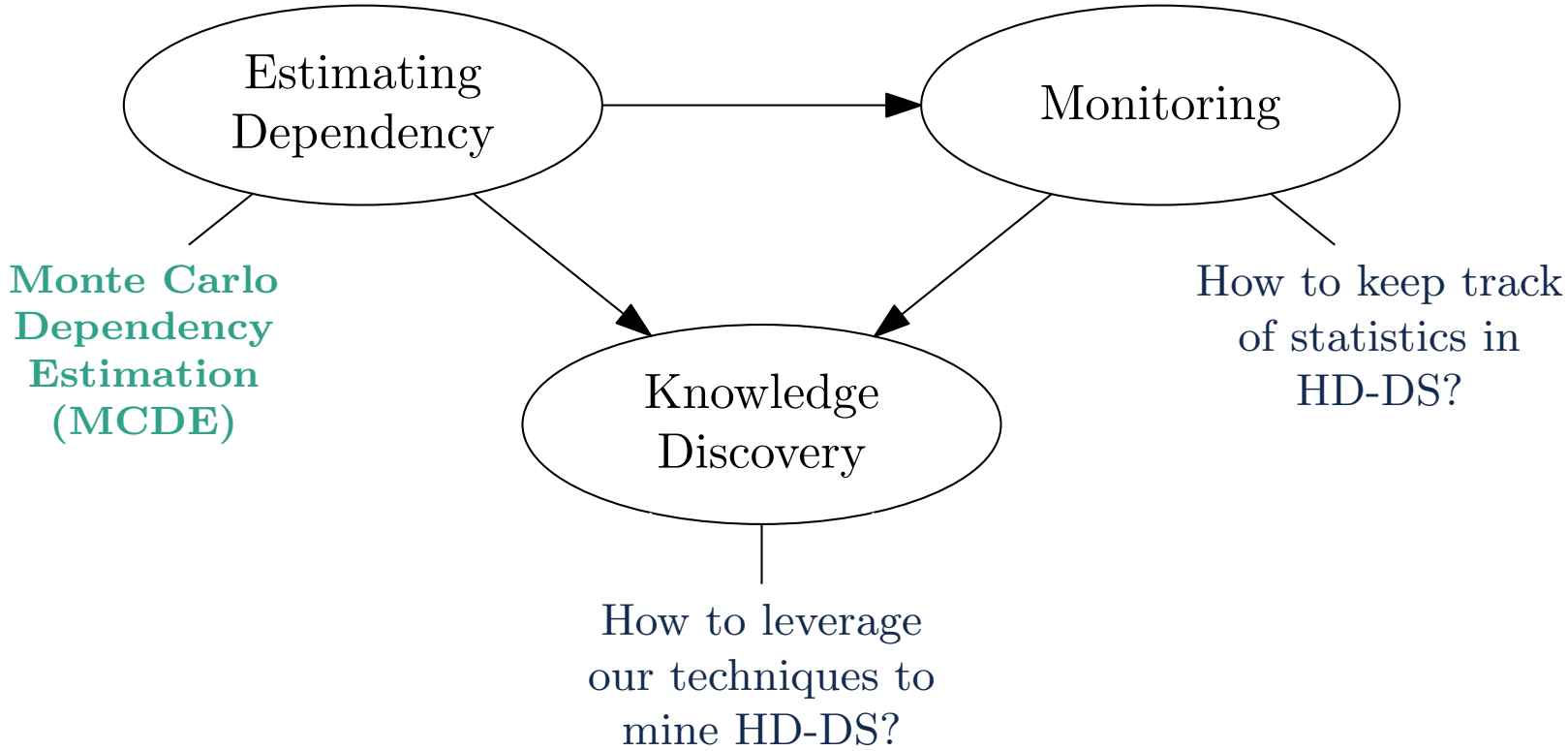

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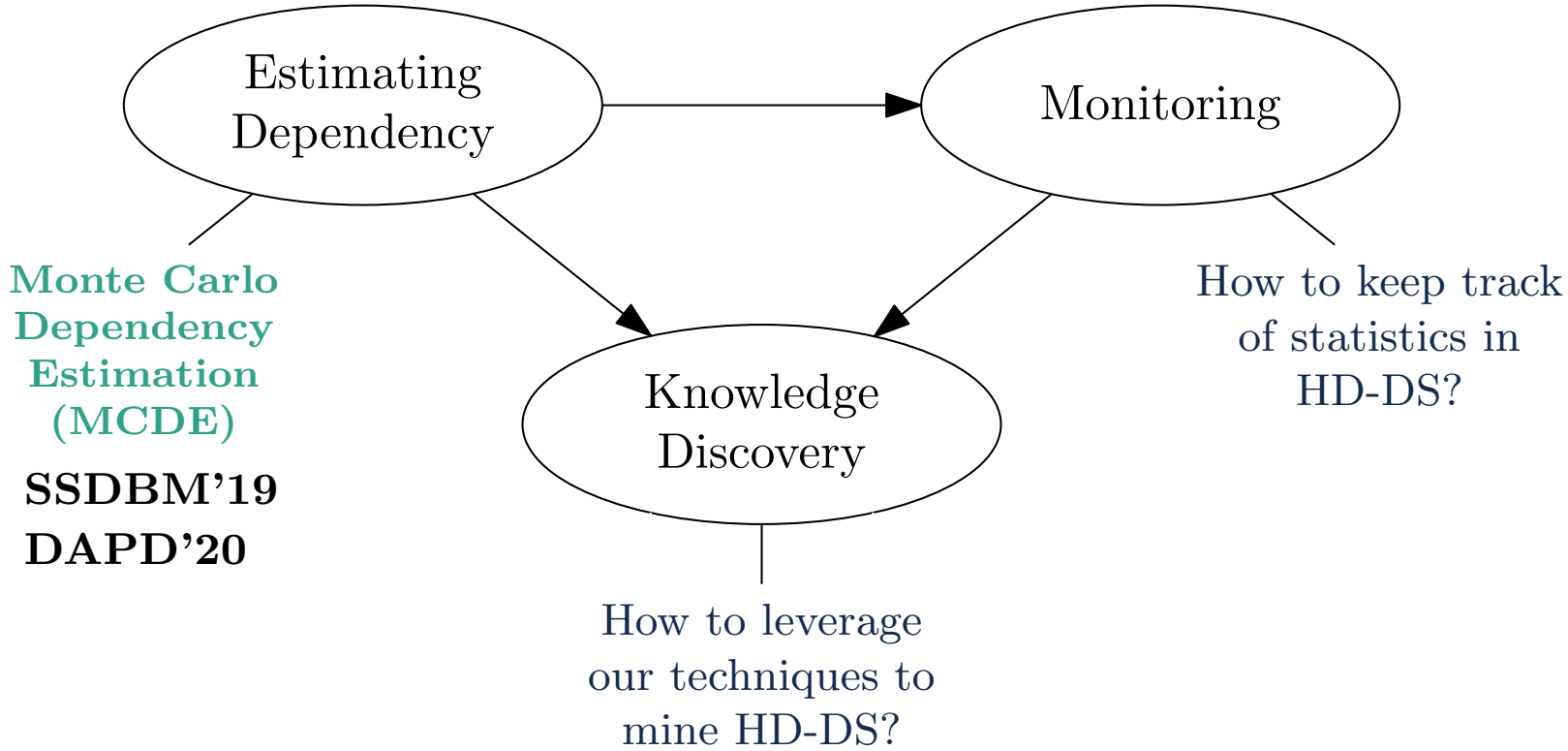

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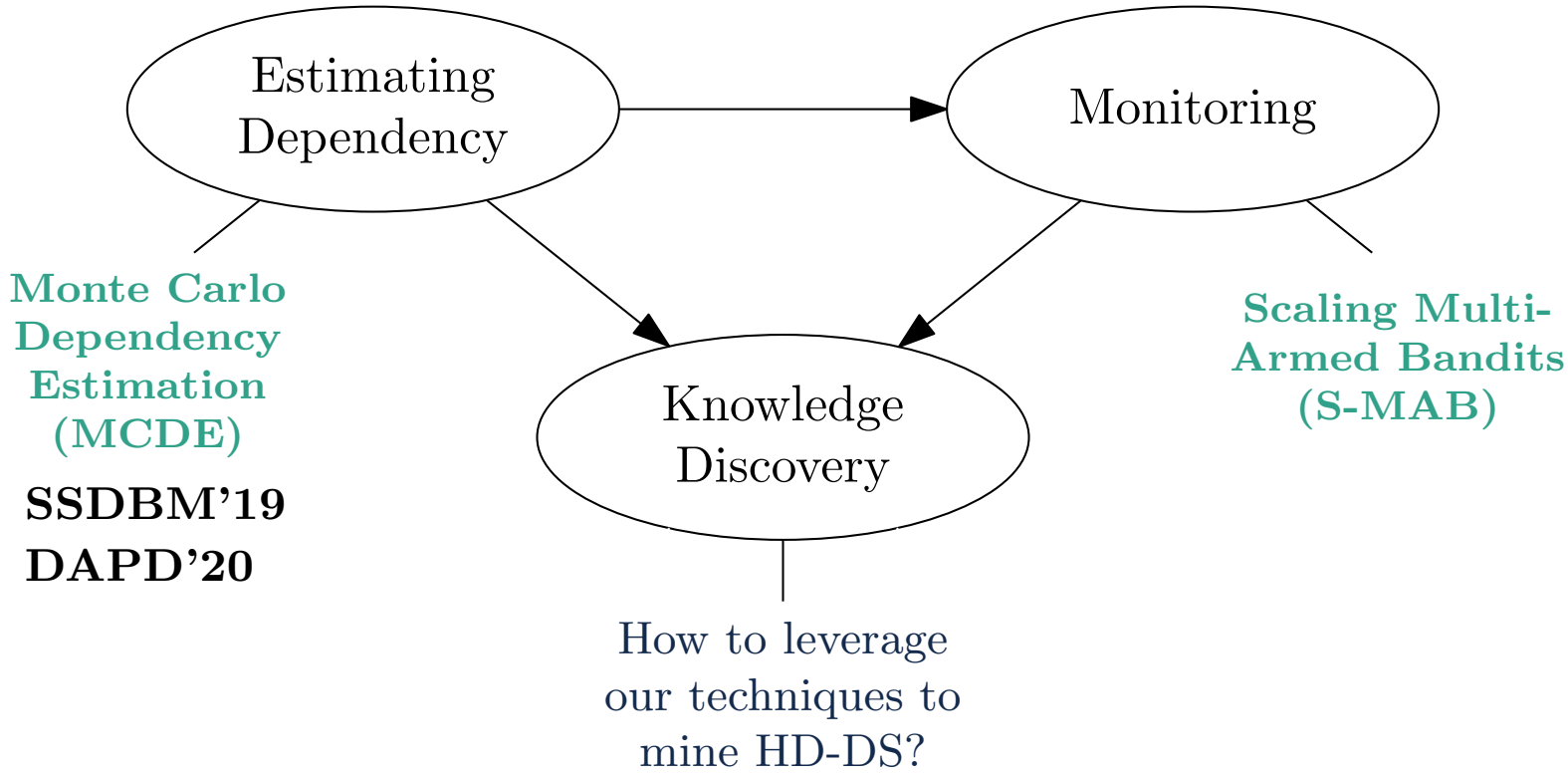

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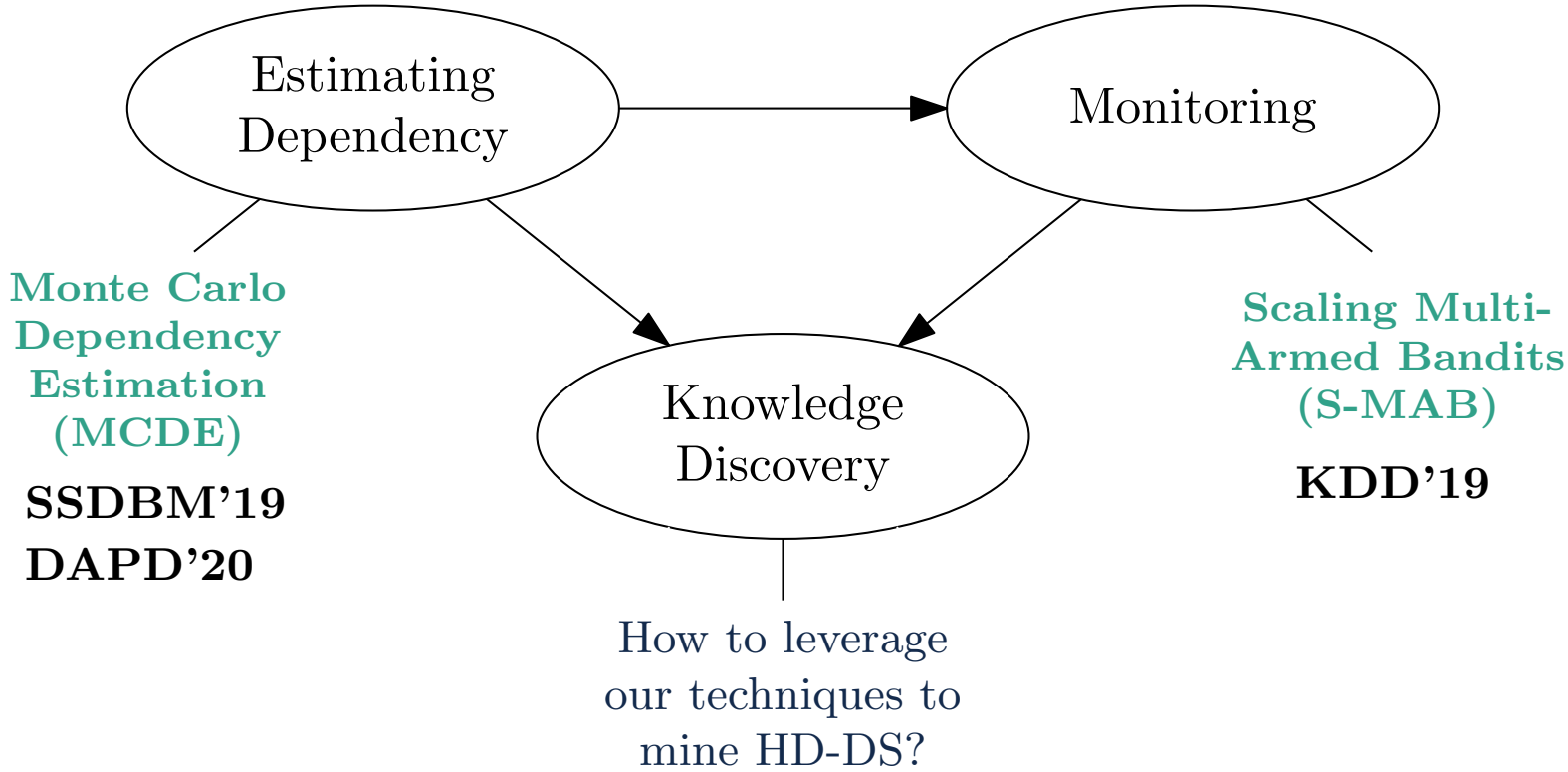

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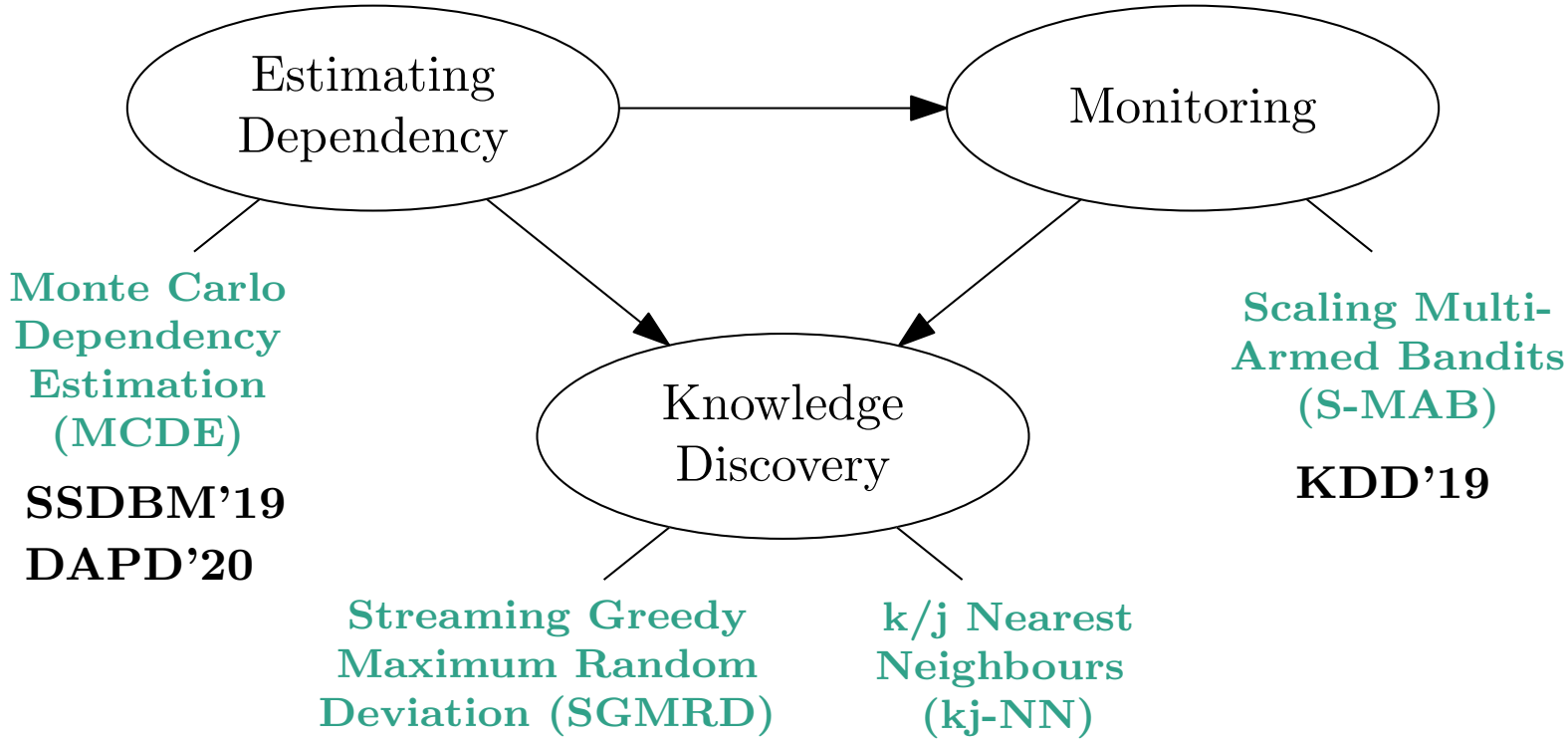

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For any given subspace $S = \{X_1, \ldots, X_d\}$:

- We see each dimension $X_i \in S$ as a random variable:

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- Then $\neg B \Rightarrow \neg A$ (non-independence)
  - Our idea: quantify $\neg B$ as $discrepancy(p_{X_i}(S), p(S|\overline{X_i})), \forall X_i \in S$
  - We propose a Monte Carlo method to approximate the *discrepancy*

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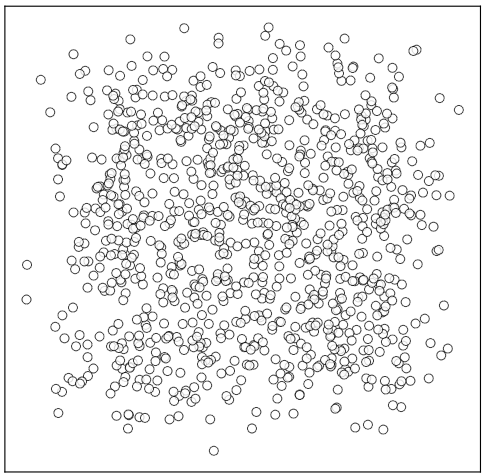

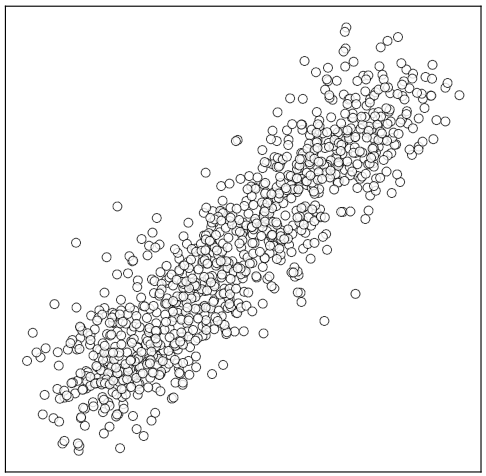

- Take a random slice
- Test $\mathcal{T}(\hat{p}_{X_i}(S), \hat{p}(S|\overline{X_i}))$
- Repeat M times
- Average:

$$\mathcal{C} = \frac{1}{M}\sum_{m=1}^{M}(1 - p\text{-}value)$$

Properties:

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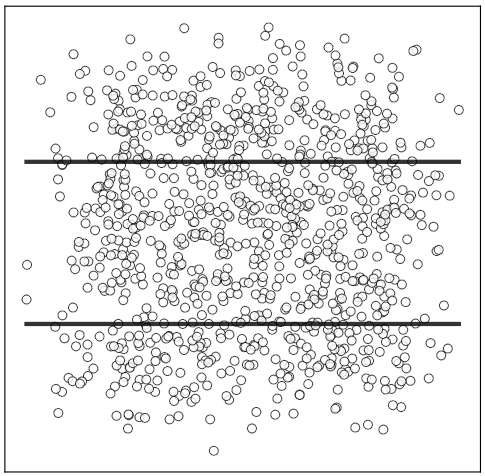

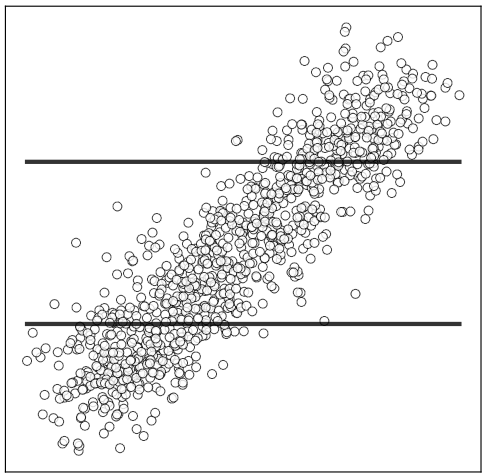

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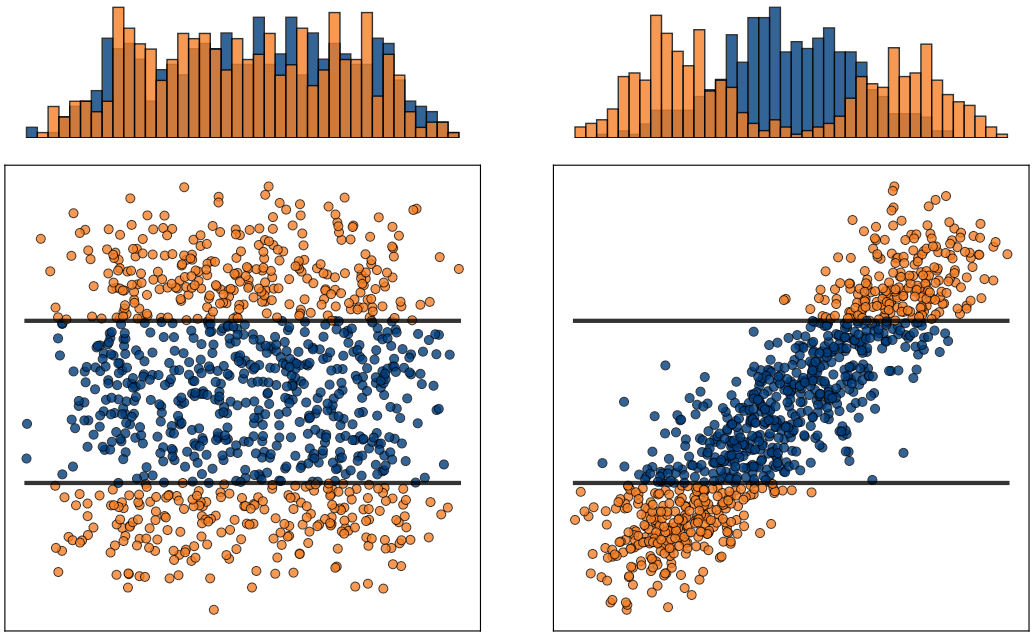

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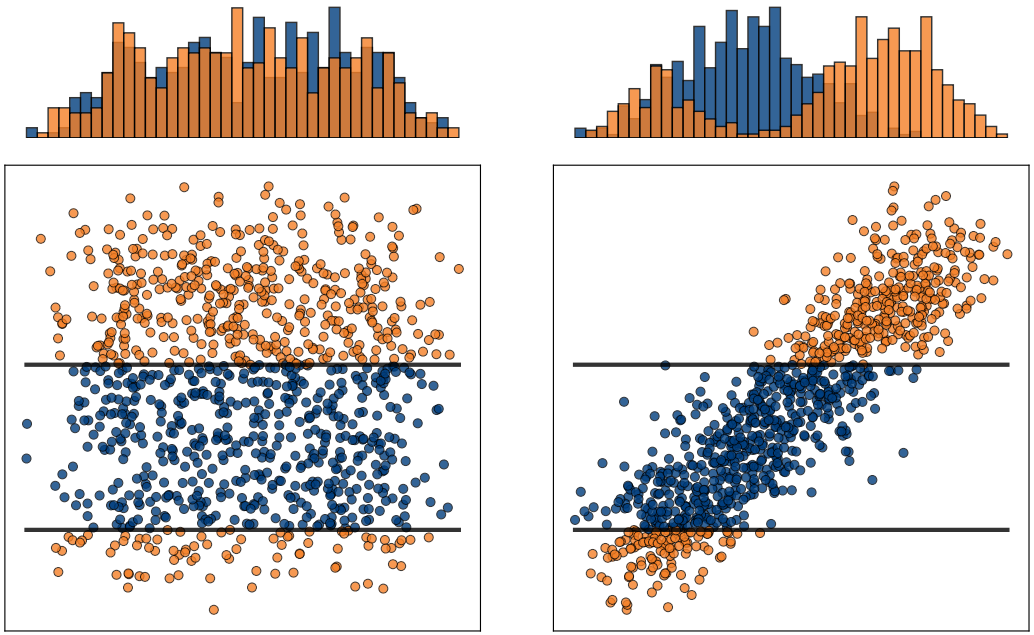

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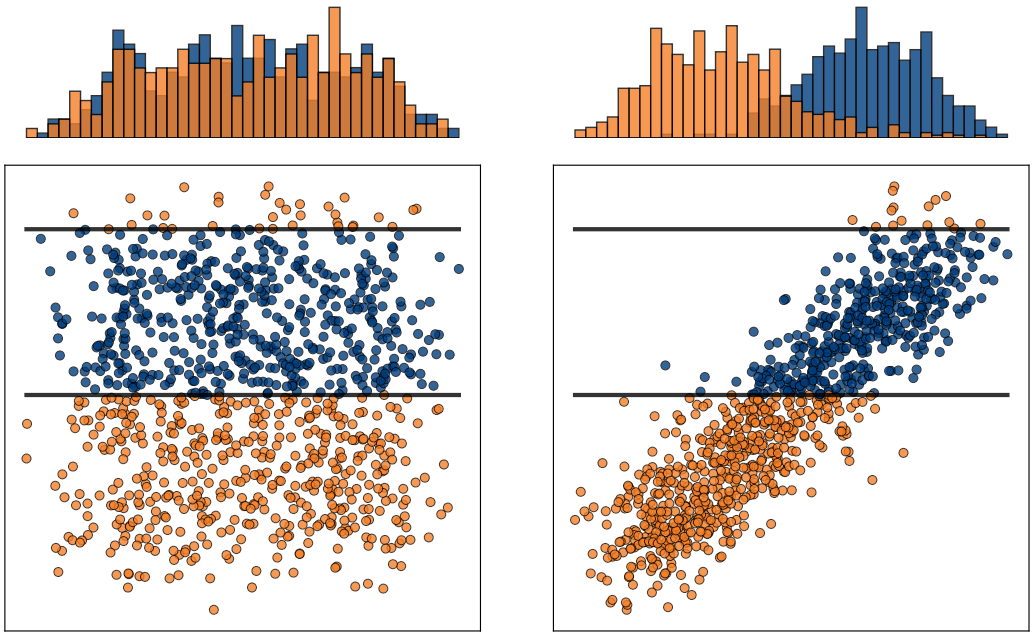

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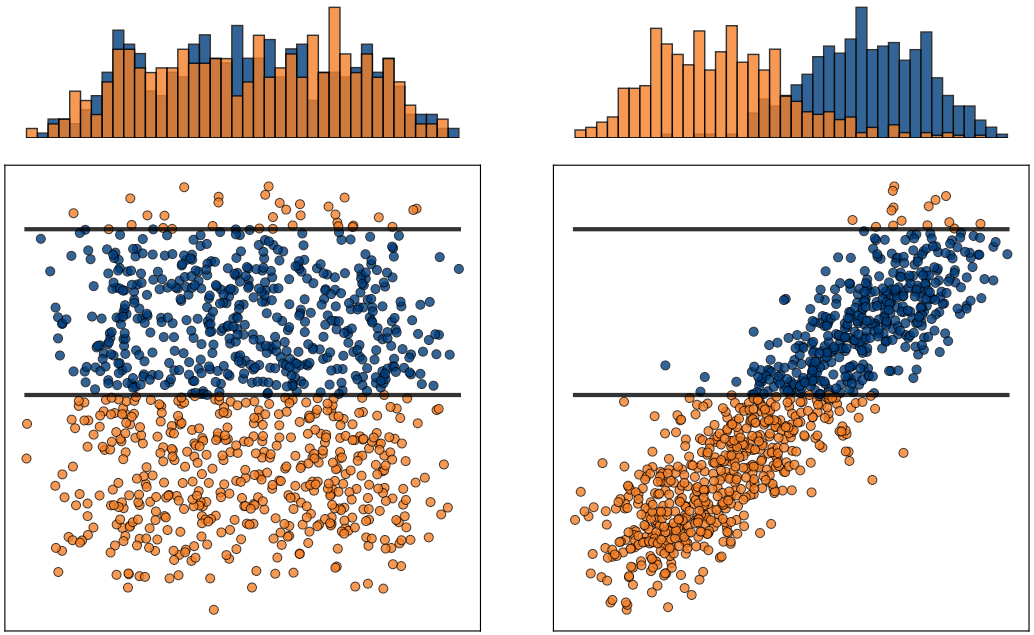

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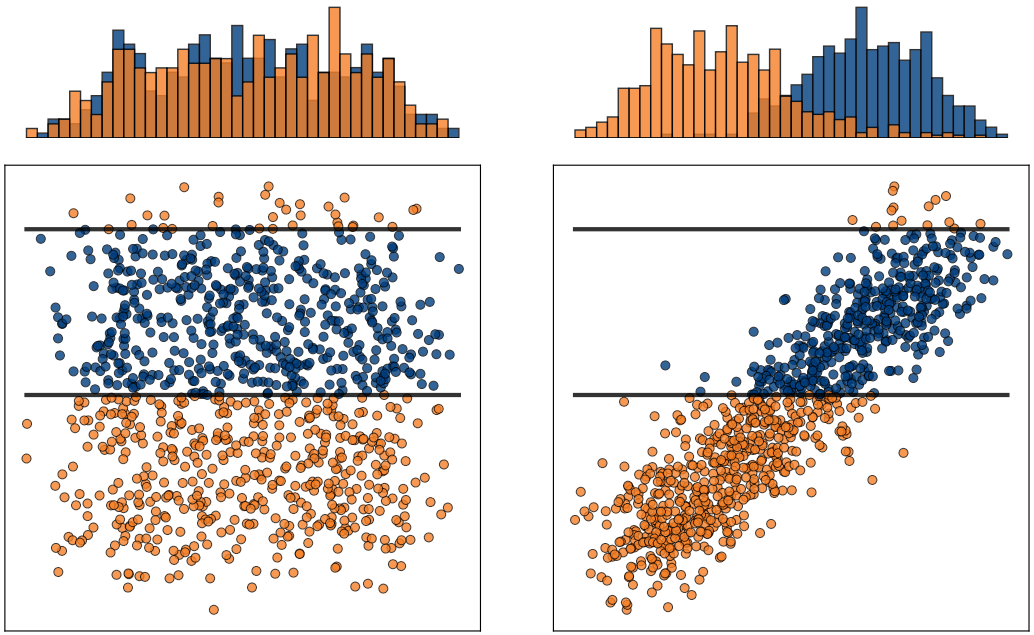

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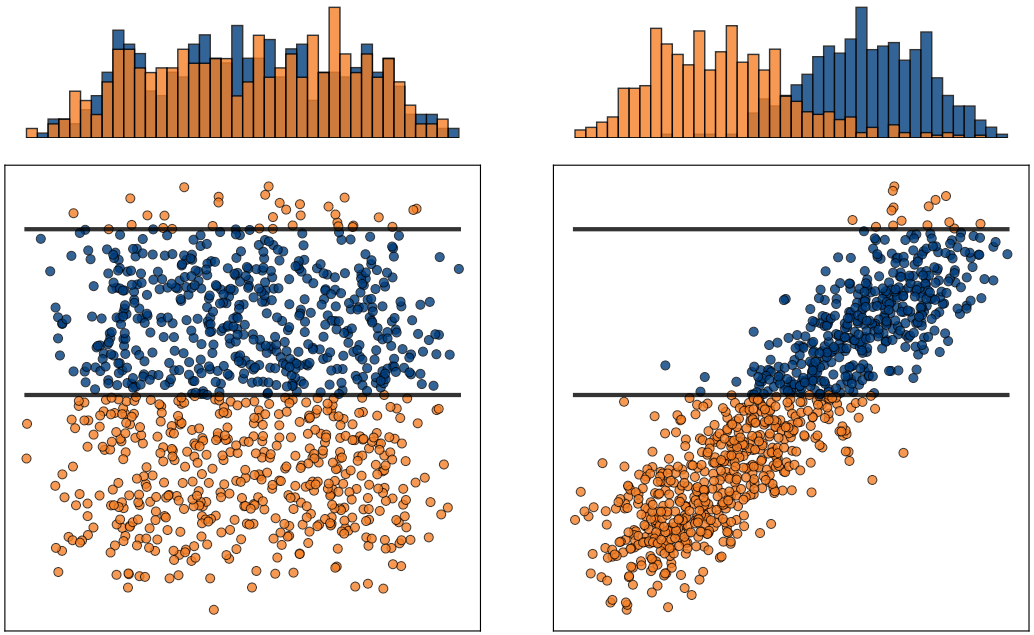

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MCDE: A General Estimation Framework

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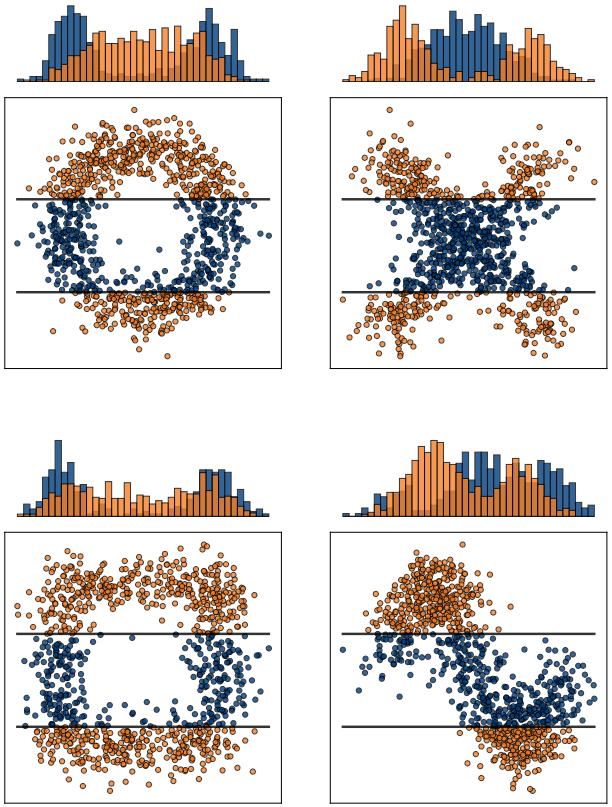
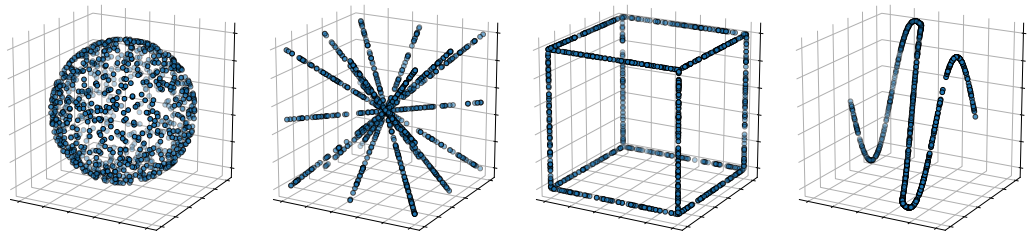


- Multivariate data



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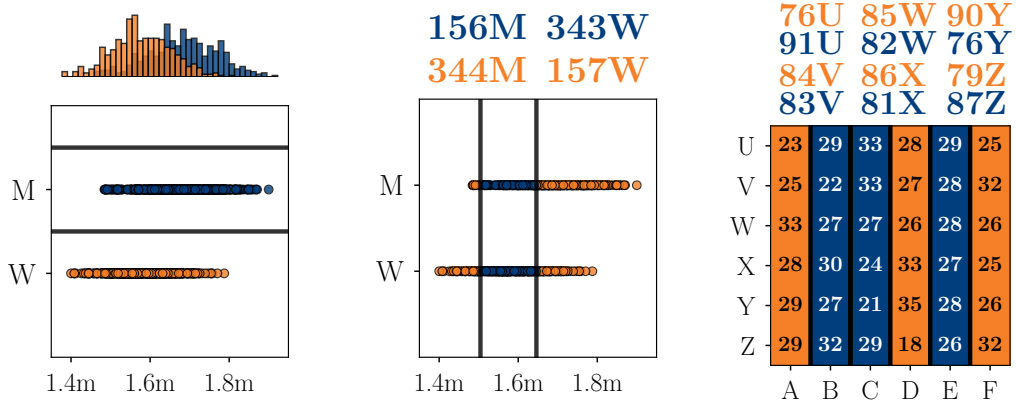

Evaluating MCDE

We systematically assess MCDE against 12 requirements.

	Efficient	Single-Scan	Adaptation	Anytime	Heterogeneity	Multivariate	General	Intuitive	Non-parametric	Interpretable	Sensitive	Robust
MS*	++	✗	✗	✗	✗	✓	✗	✓	✓	✓	✗	✓
TC**	-	✓	✓	✓	✗	✓	✓	✗	✓	✗	✓	✗
II***	--	✓	✓	✓	✗	✓	✗	✗	✓	✗	✗	✗
CMI†	+	✗	✗	✗	✗	✓	✗	✗	✓	✗	✗	✗
MAC‡	--	✗	✗	✗	✗	✓	✗	✗	✓	✗	✗	✓
UDS‡‡	-	✗	✗	✗	✗	✓	✗	✗	✓	✗	✗	✓
HiCS$	+	✗	✗	✓	✗	✓	✓	✗	✓	✗	✗	✗
MCDE	++	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓

* [SS07], ** [Wat60], *** [McG54], † [NMV+13], ‡ [NMV+14], ‡‡ [NMV16], $ [KMB12]

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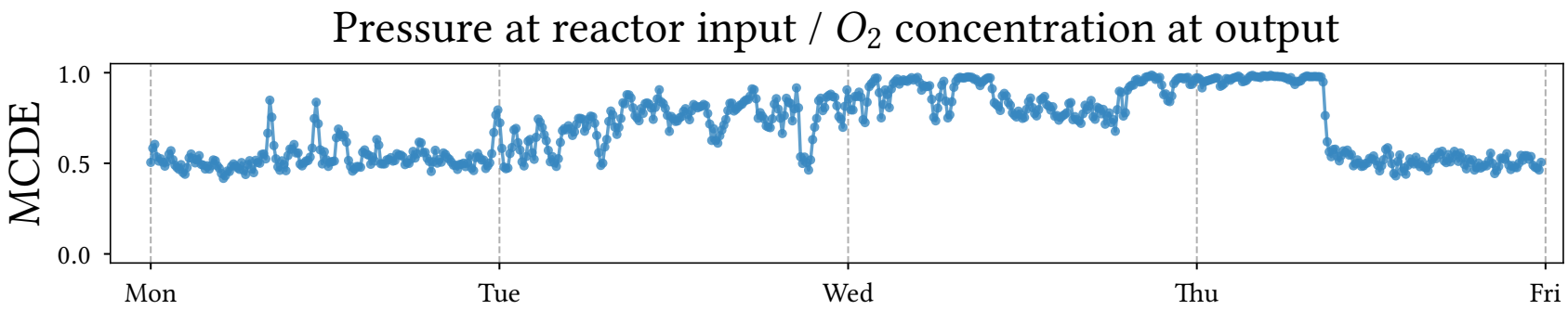

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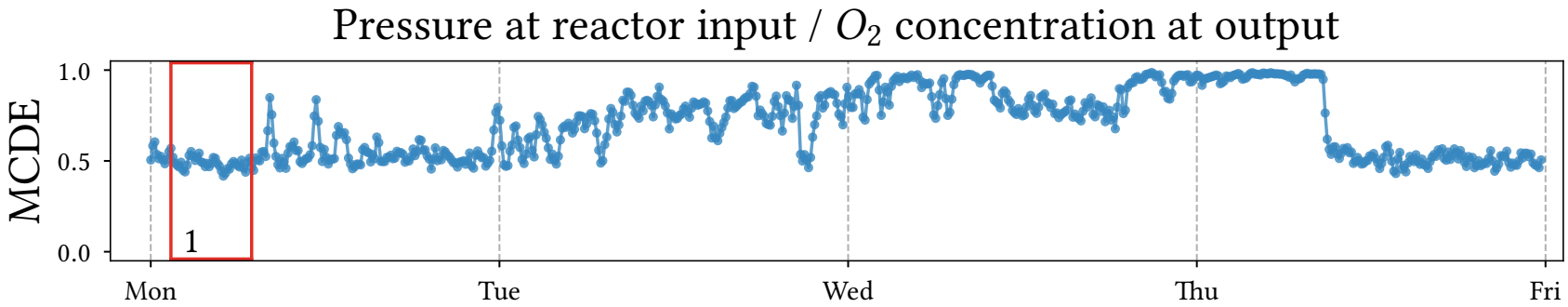

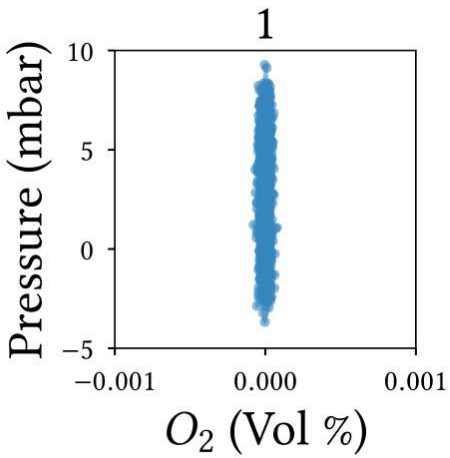

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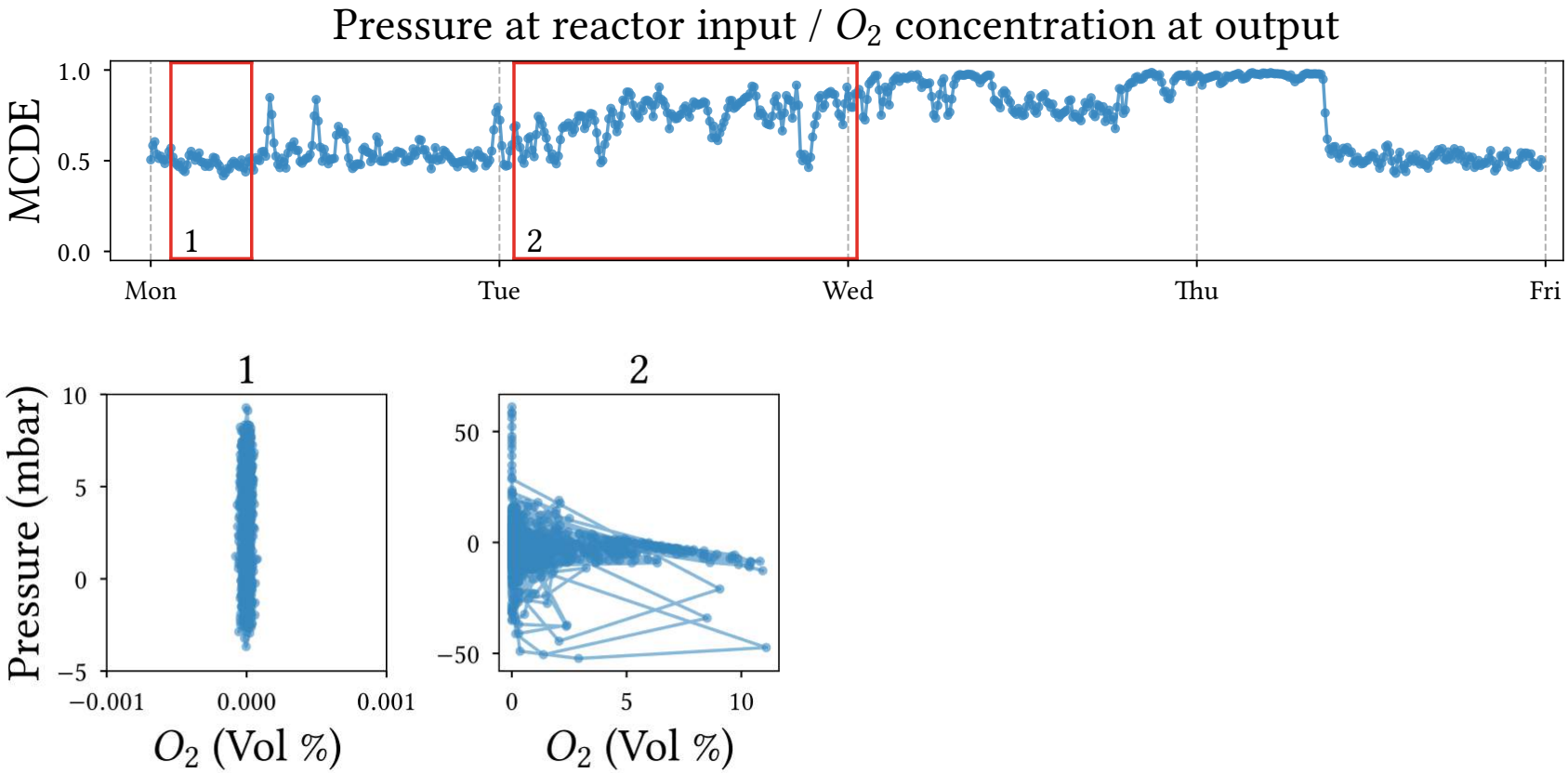

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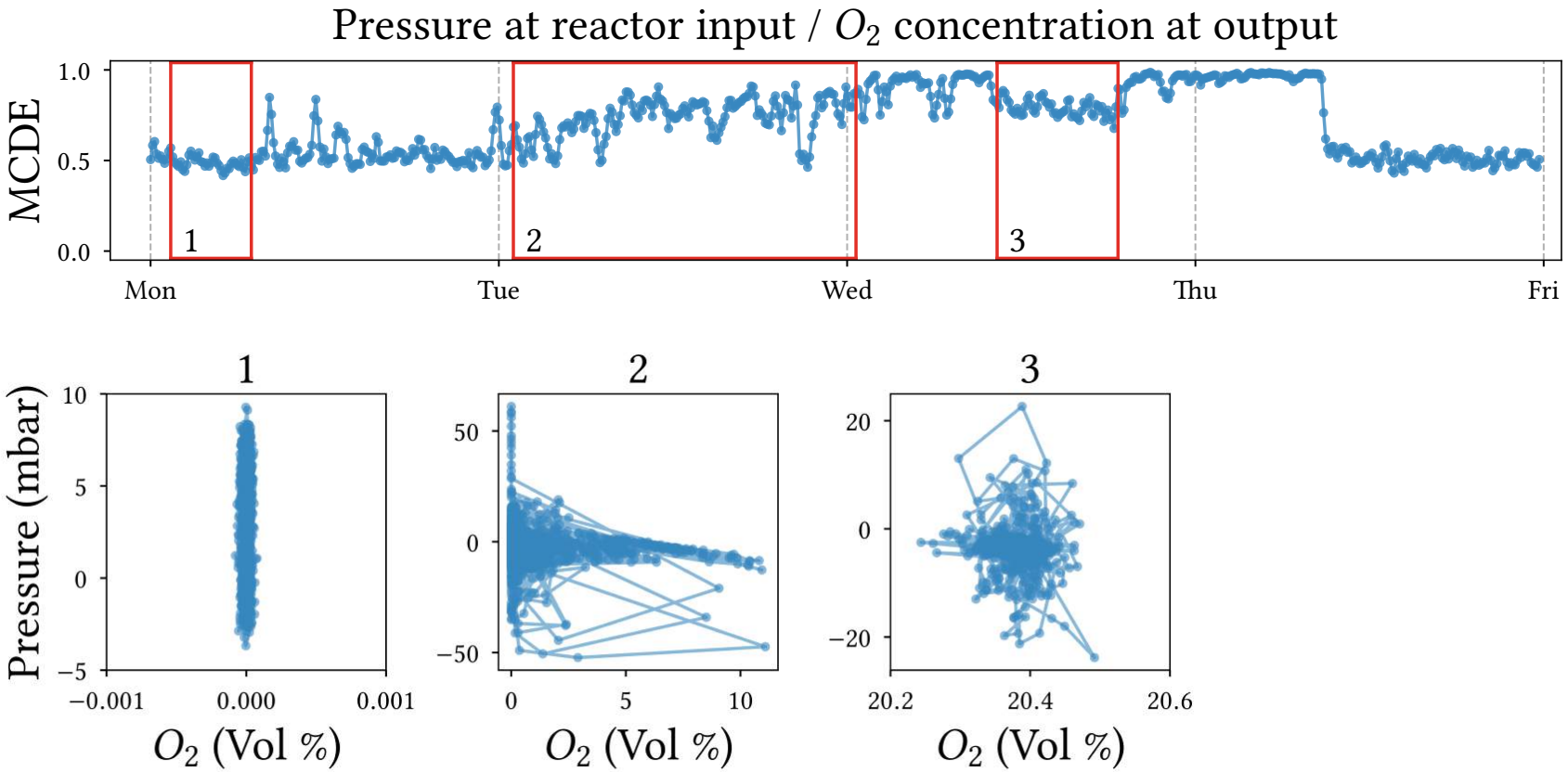

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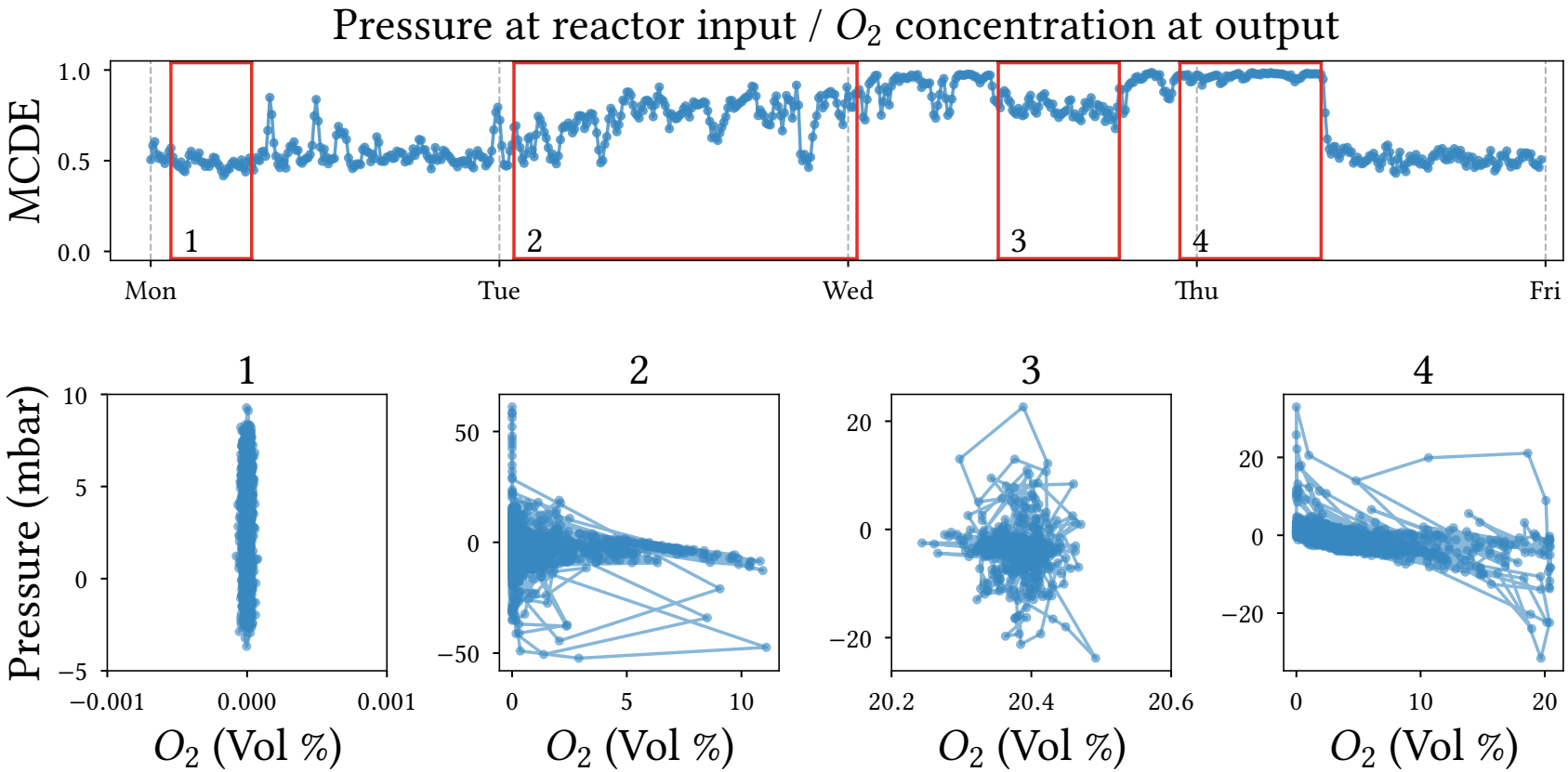
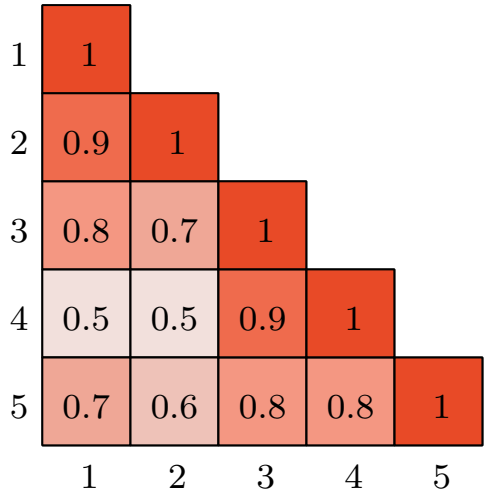


From Estimating to Monitoring

Now, we are able to estimate dependency in HD-DS.



- However, there are too many pairs/subspaces
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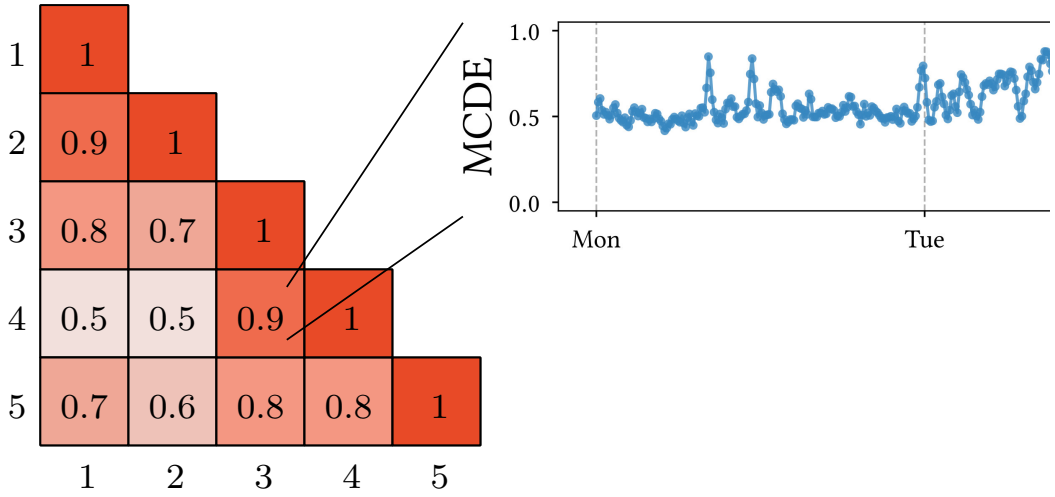

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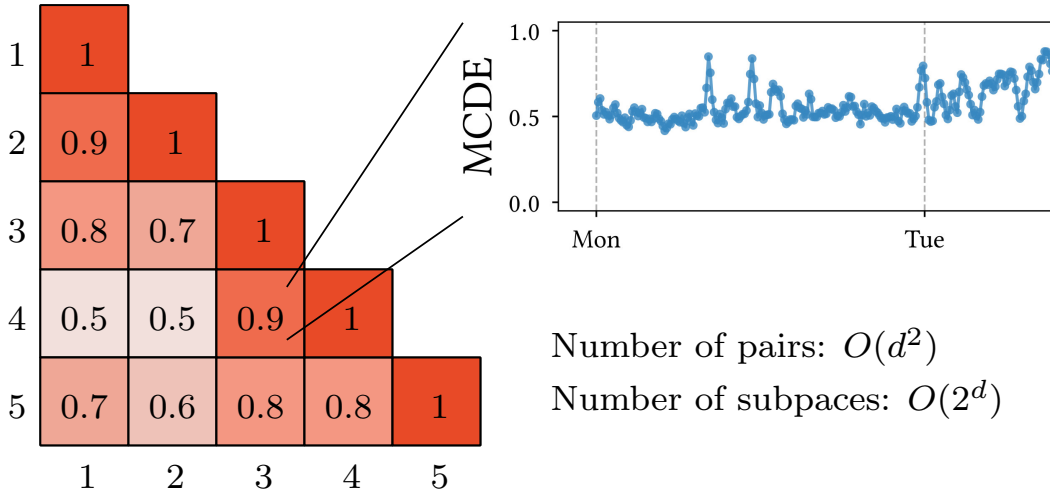

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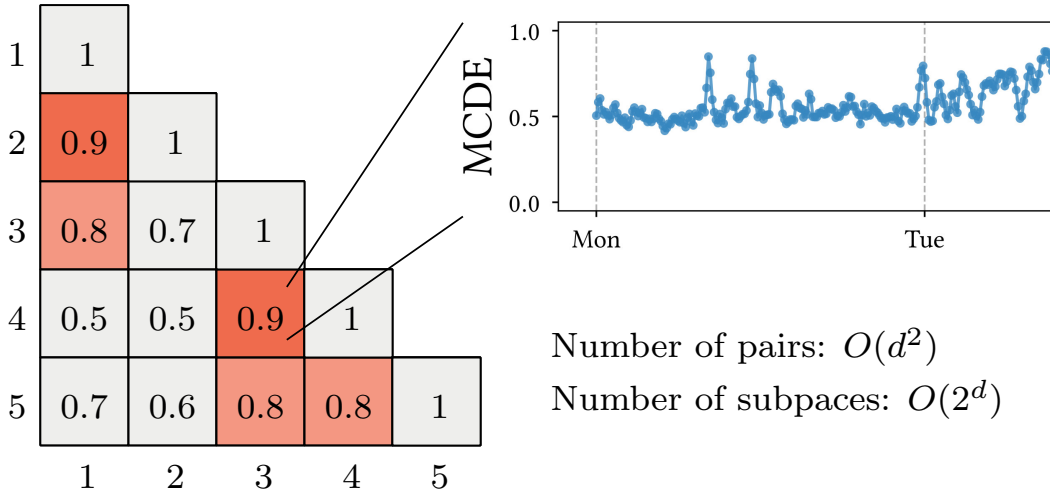

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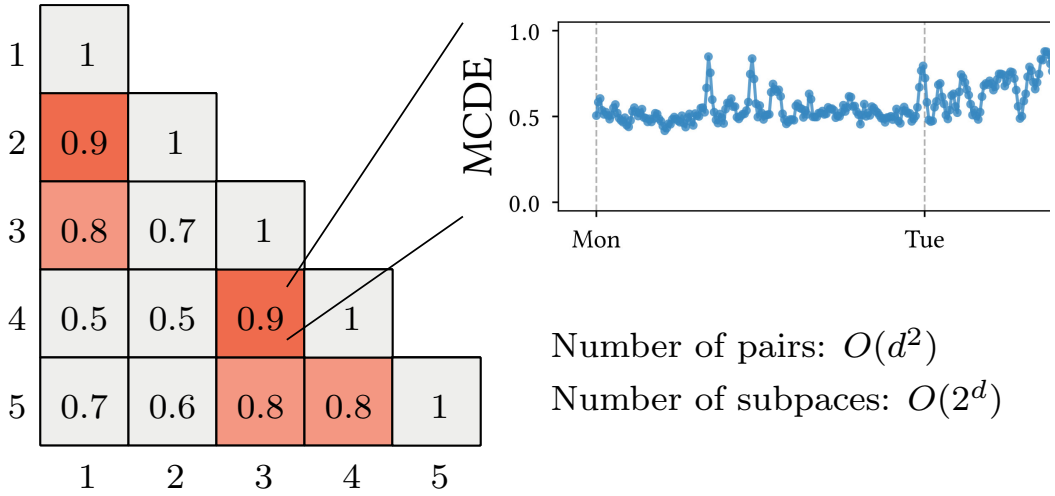

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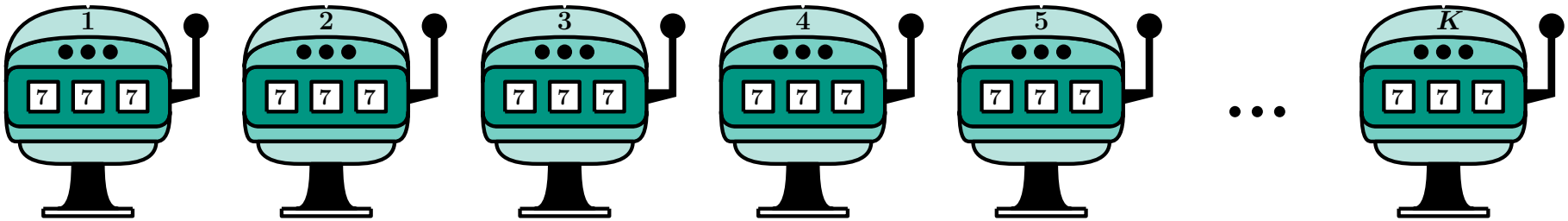

To maximise our gain, we need to find:

- Which arms are the best?
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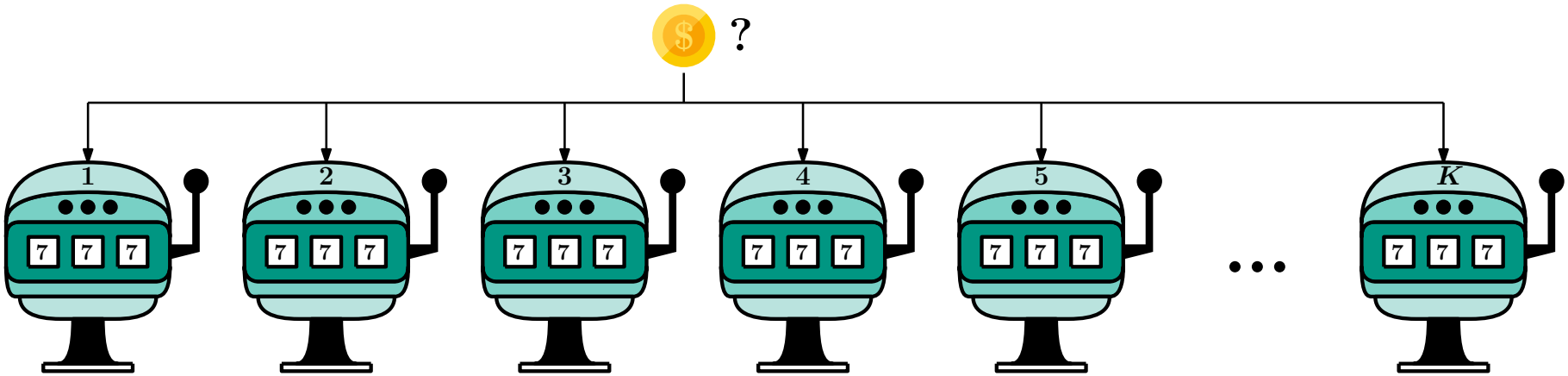

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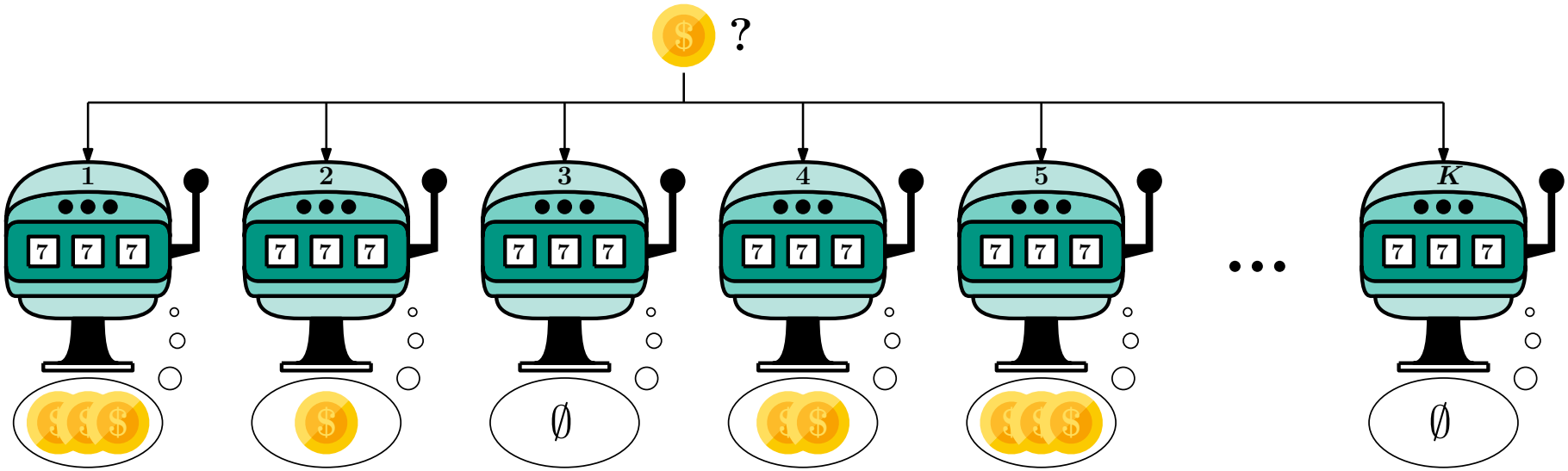

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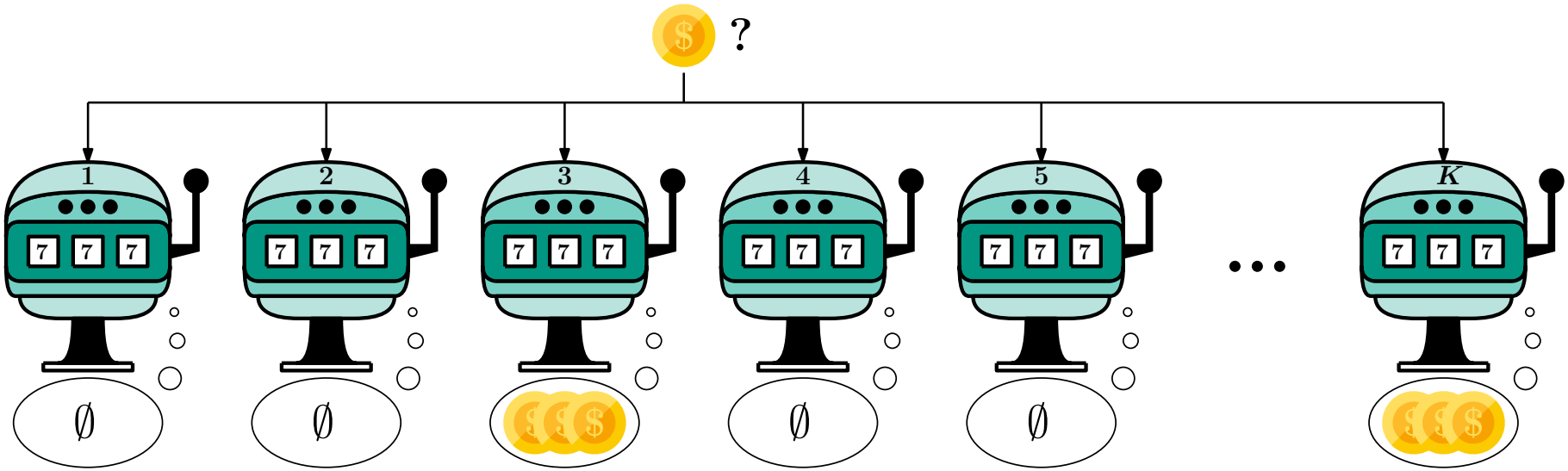

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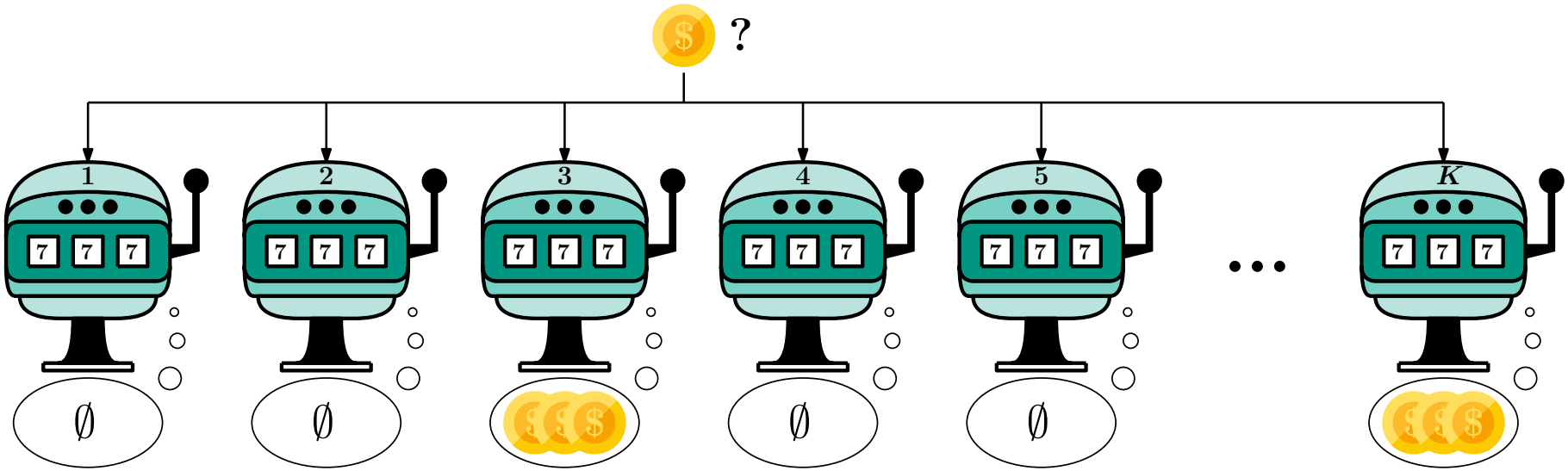

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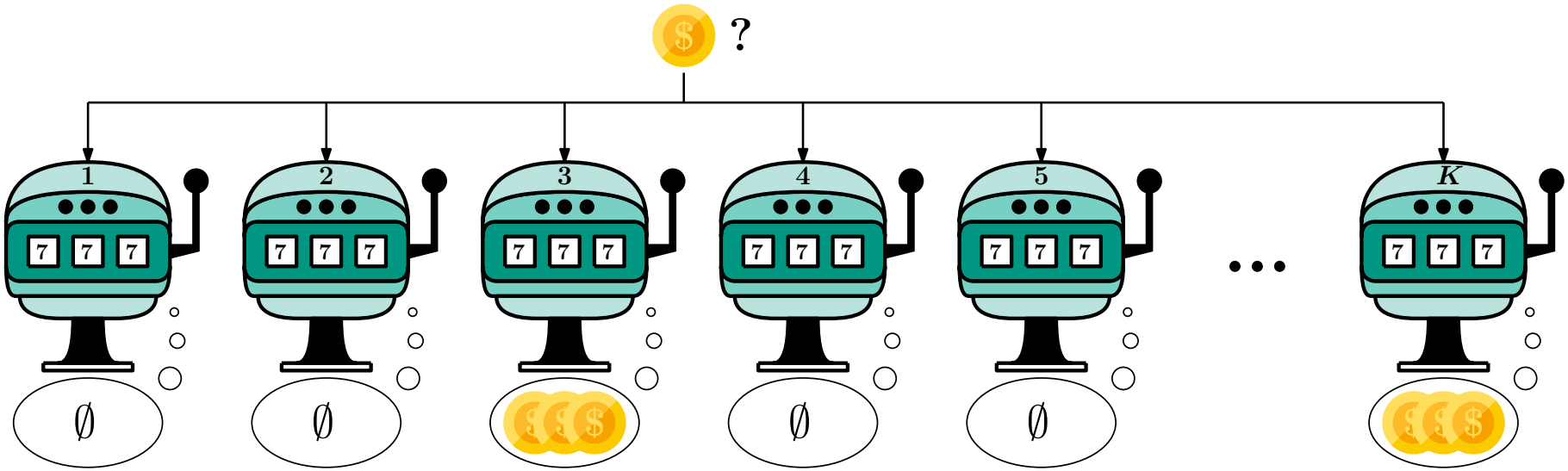
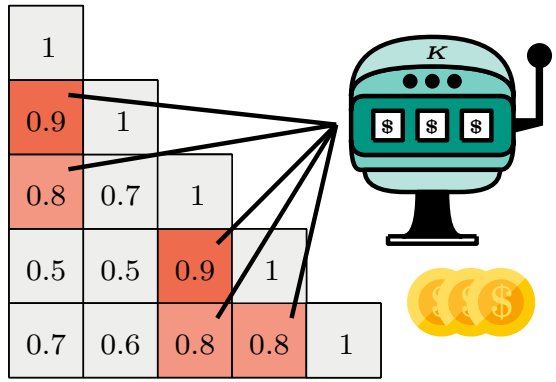


To maximise our gain, we need to find:

- Which arms are the best?
- How many arms to play?
- When to adapt?



Bandit Models

Problem: Existing models do not capture our setting

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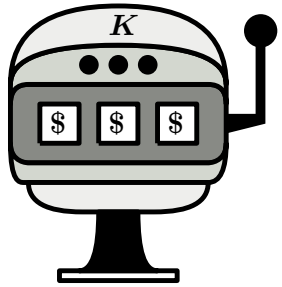

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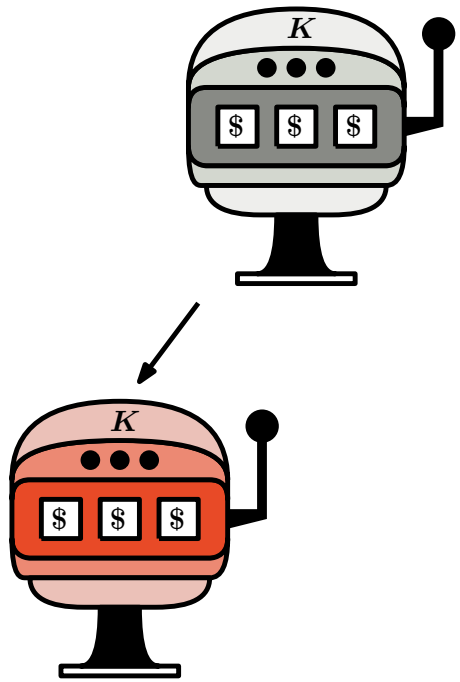

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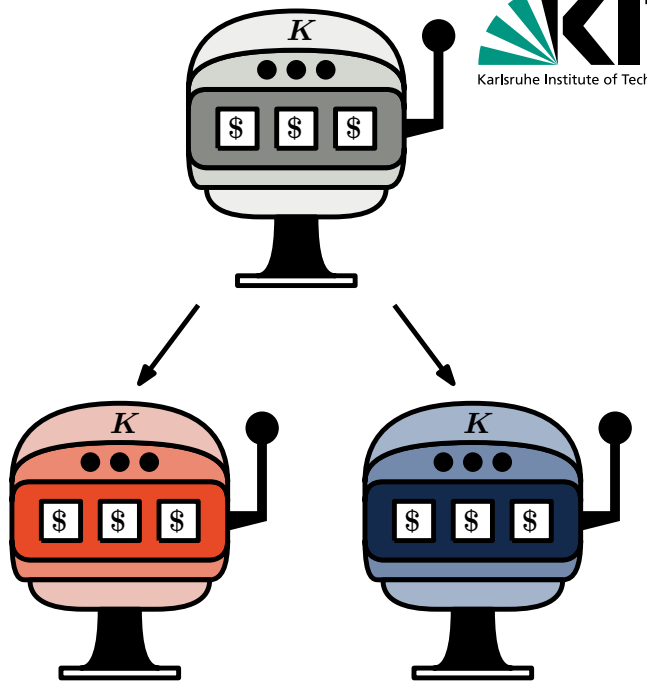

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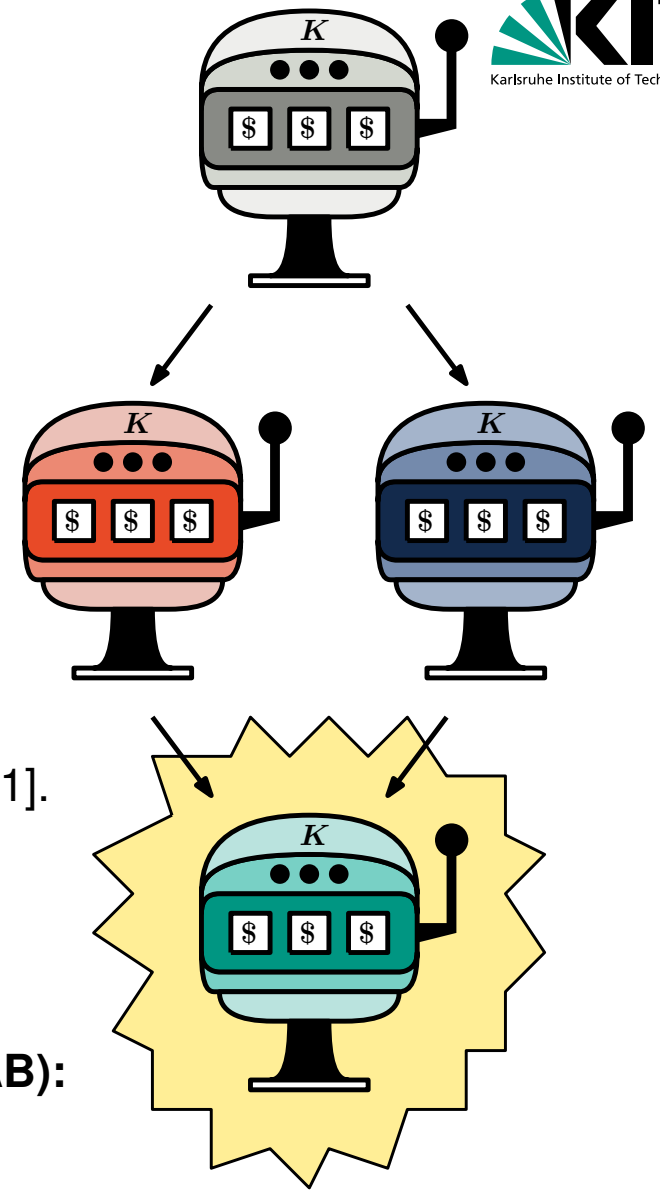

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$$\underbrace{\max_{I_t \subset [K]}}_{\text{Set of arms}} \overbrace{\sum_{i \in I_t} S_i(t)}^{\text{Sum of rewards}} \quad s.t. \quad \underbrace{\eta_t = \frac{\sum_{i \in I_t} \mu_i}{|I_t|}}_{\text{Average expected reward}} > \overbrace{\eta^*}^{\text{Efficiency}} \tag{1}$$

If the player always chooses the best arms, then the problem is equivalent to finding an optimal number of plays L^*:

$$L^* = \max_{1 \leq L \leq K} L \quad s.t. \quad \underbrace{\frac{\sum_{i=1}^{L} \mu_i}{L}}_{\substack{\text{Average expected reward} \\ \text{from the top-L arms}}} > \eta^* \tag{2}$$

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General Scaling Multi-Armed Bandit

Two components for success: $\overbrace{\text{finding the top-arms}}^{\text{Existing bandits}} + \overbrace{\text{finding } L^*}^{\text{New !}}$

At each round $t = 1, \dots, T$:

- 1. The player chooses I_t with $|I_t| = L_t$, and observes a reward vector X_t
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There exists many approaches for steps $1, 2$:

- Multiple-Play Thompson Sampling (MP-TS) [Tho33, KKM12, KHN15]
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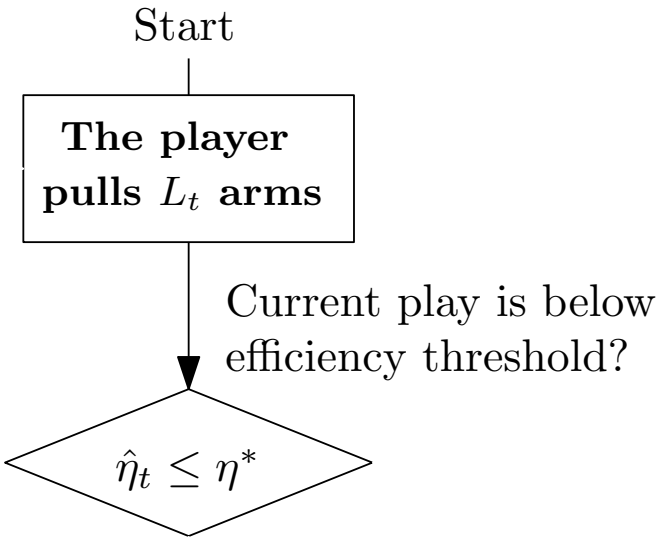

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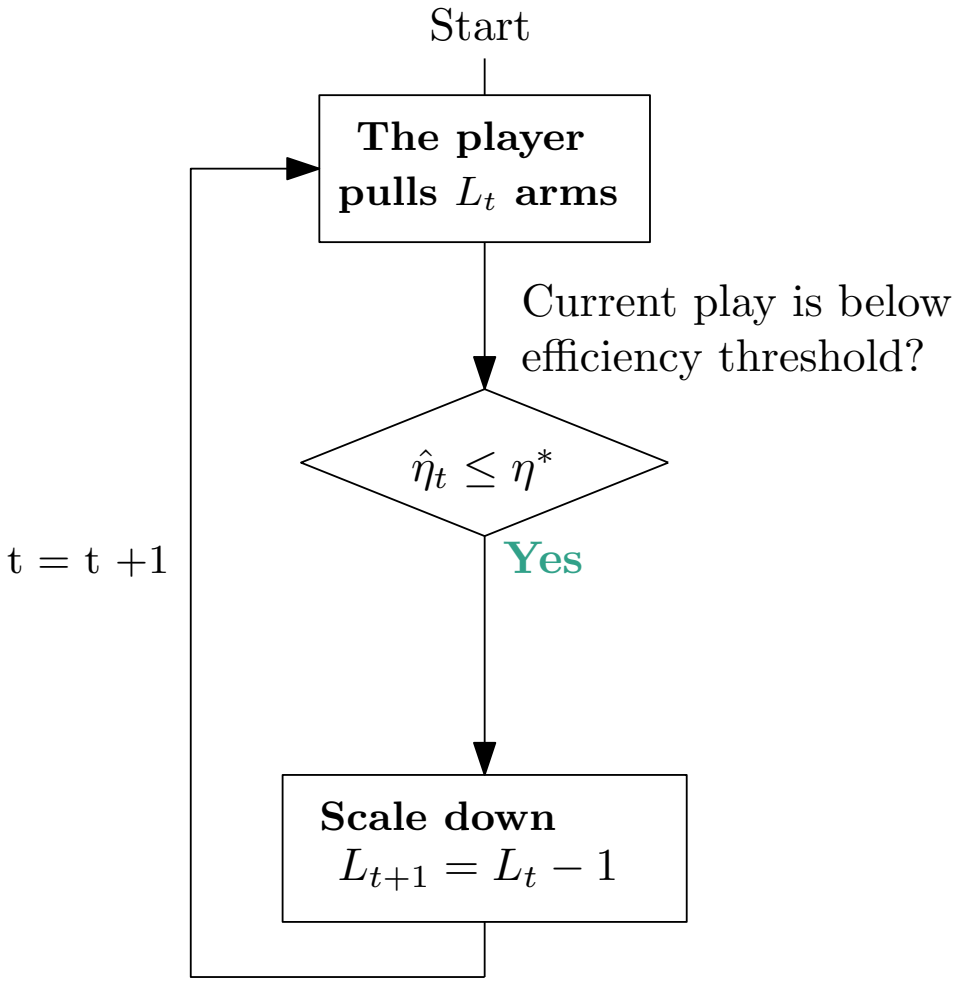

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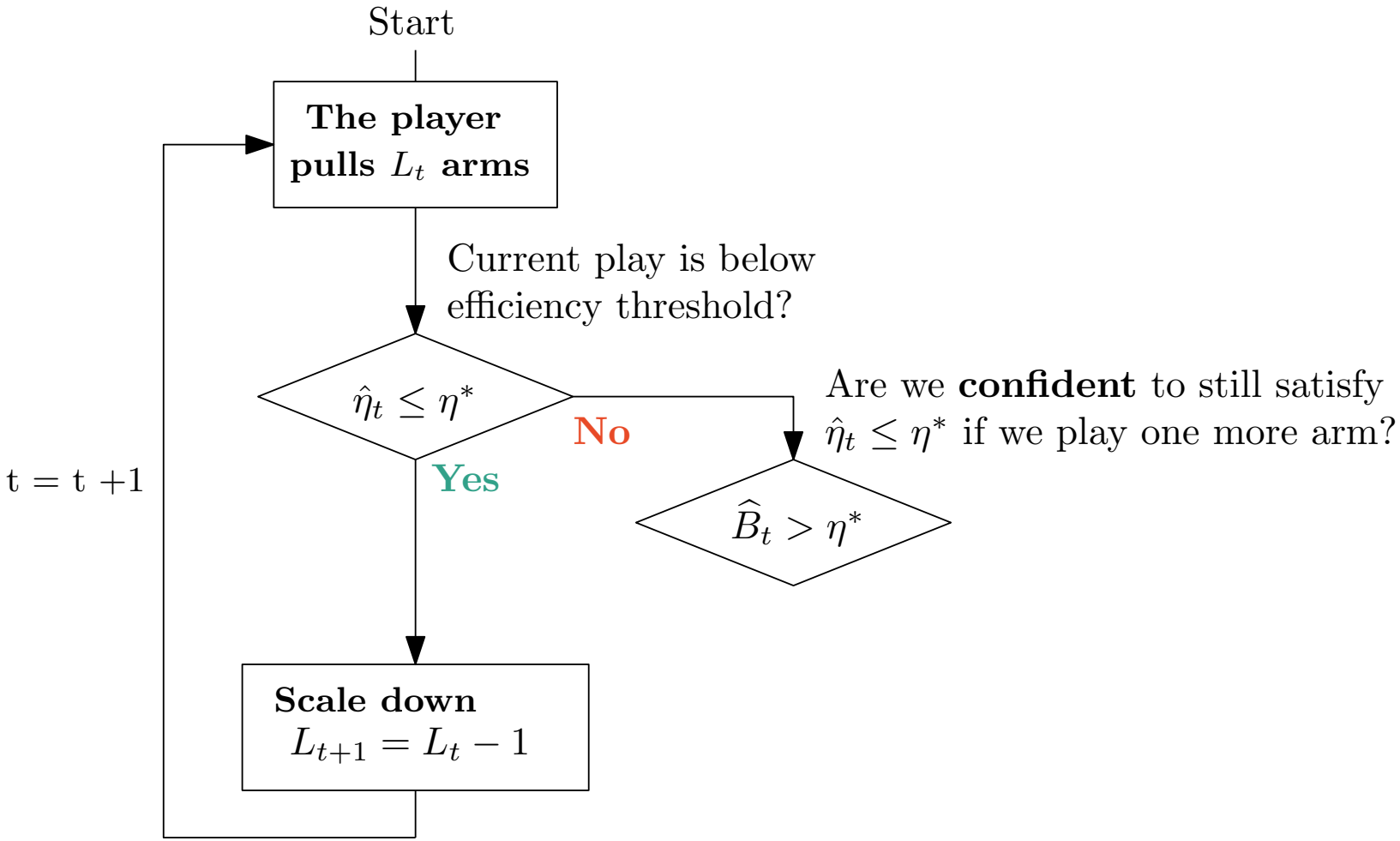

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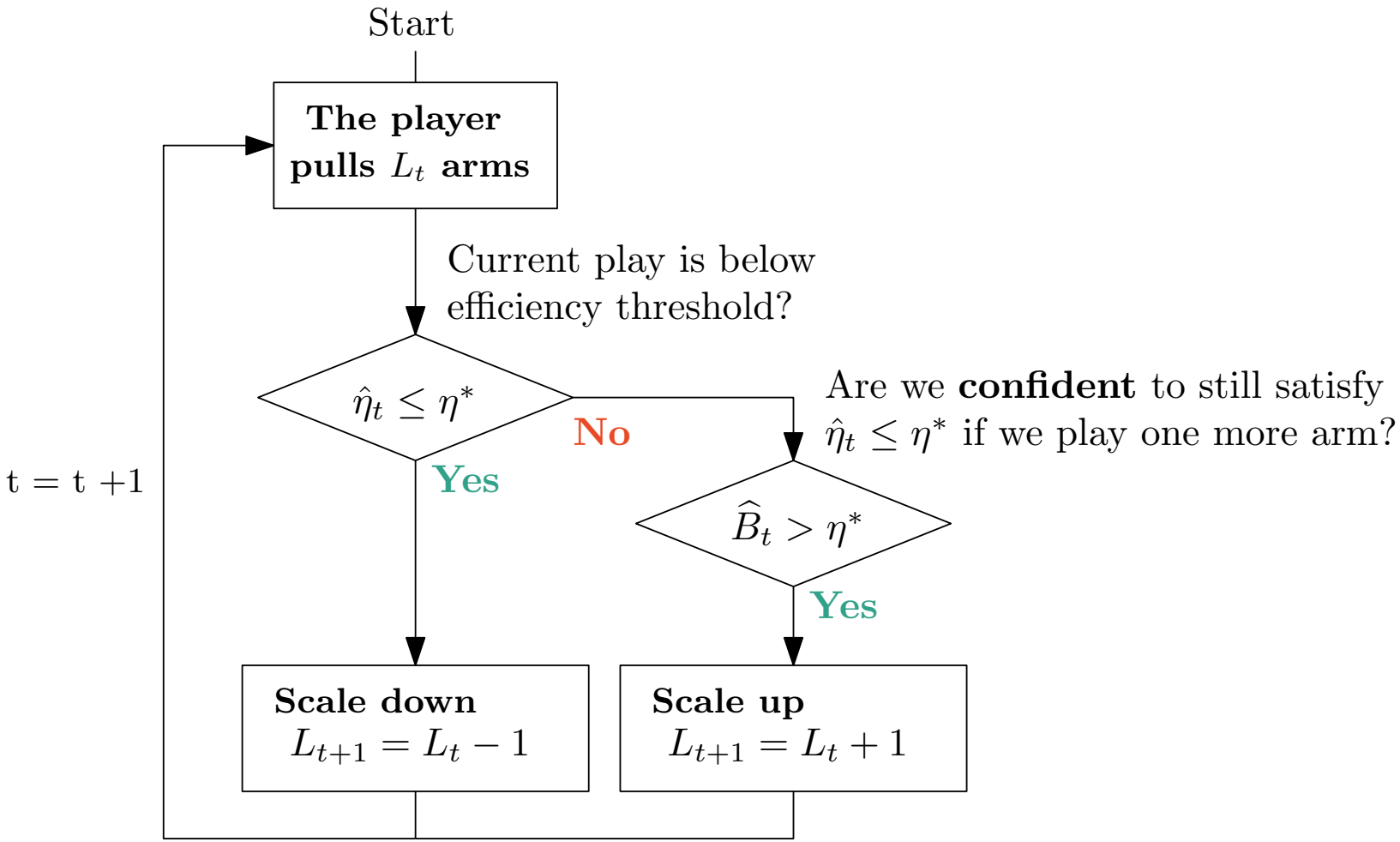

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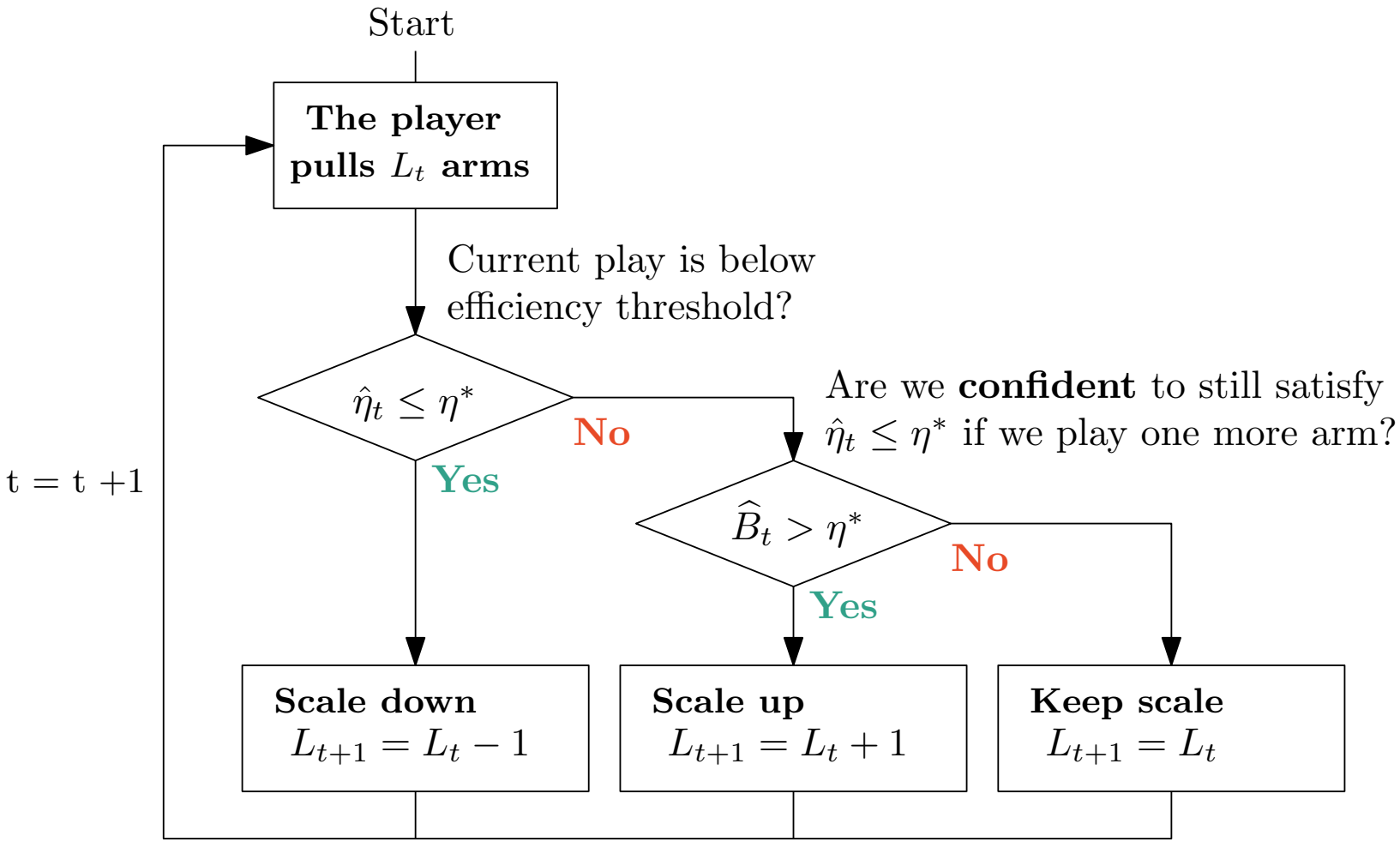

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We want to minimise two notions of regret:

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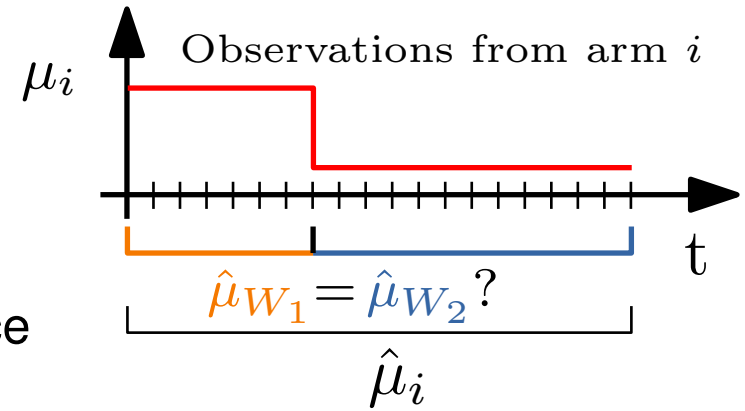
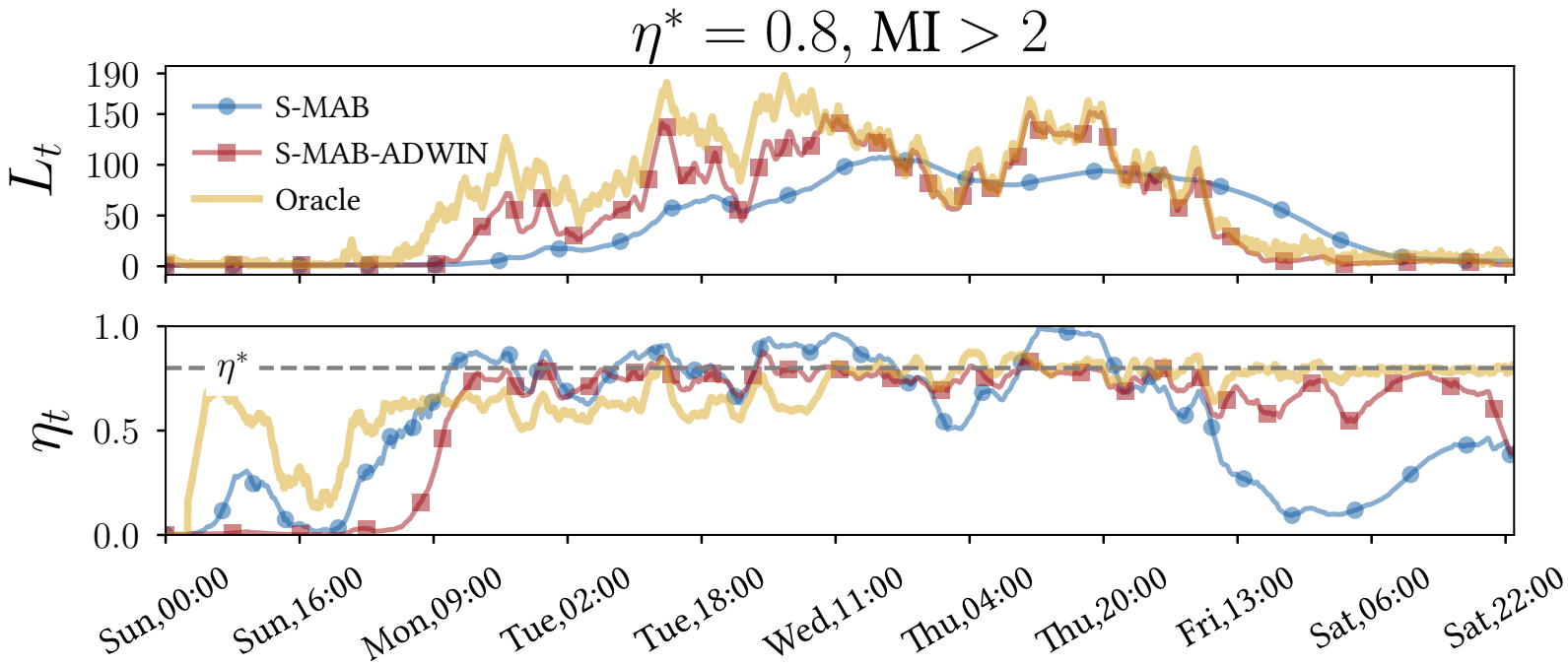


Deploying S-MAB @ Bioliq

- Bioliq: Monitoring MI between 20 sensors, 1 week of data



- S-MAB-ADWIN can adapt to non-static streams !

Monitoring $\rightarrow$ Knowledge Discovery

Subspace Search in Data Streams

- Find at any time, a set of “high-quality” subspaces
  - High-quality subspaces reveal patterns: clusters, outliers, . . .
  - Correlation/Dependency is a good proxy for such “quality”
- They are difficult to find, because we consider HD-DS:
  - There are so many subspaces
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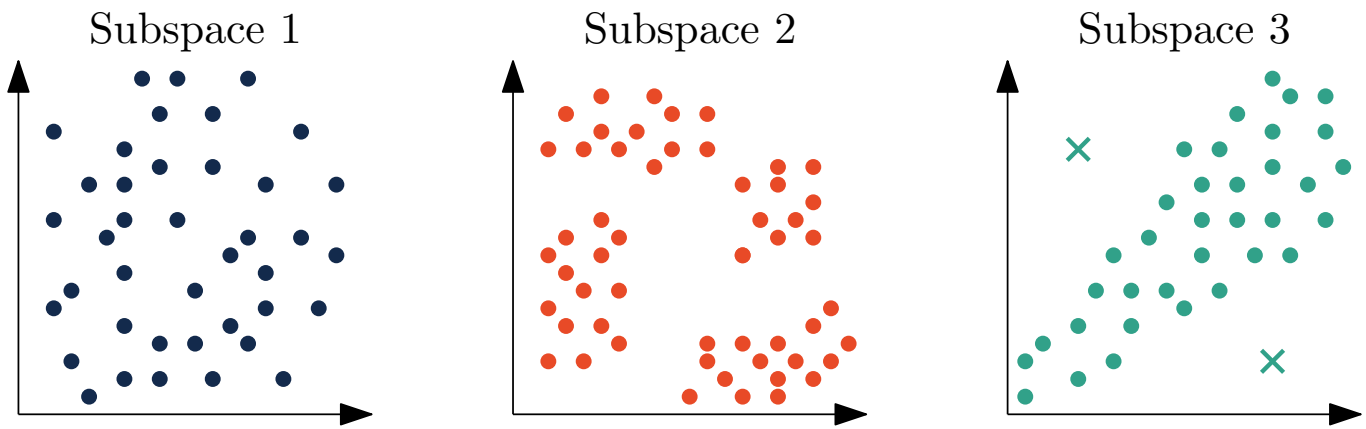

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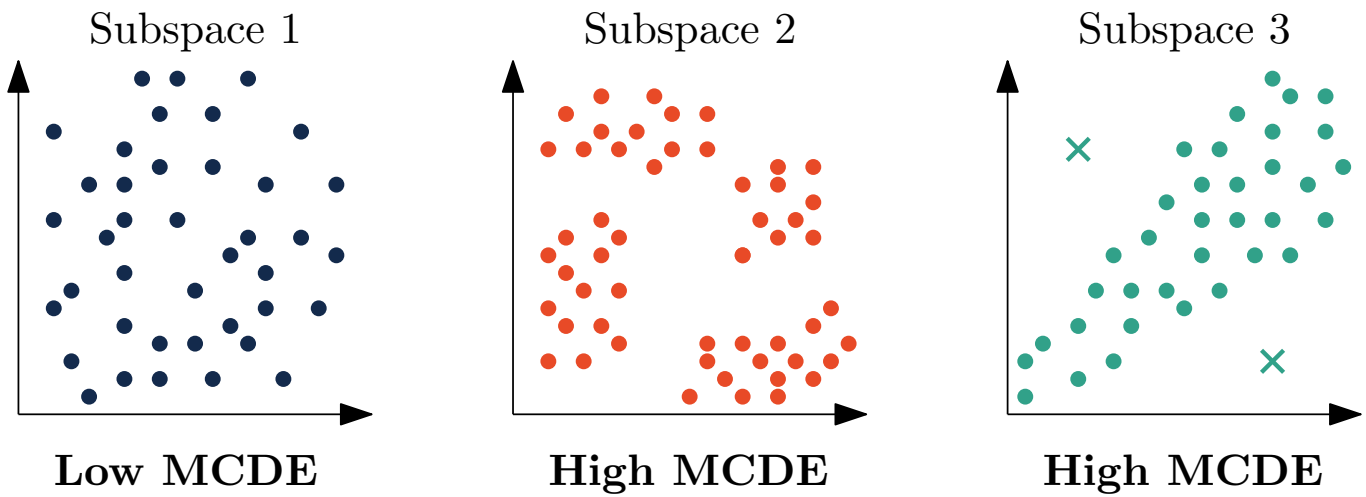

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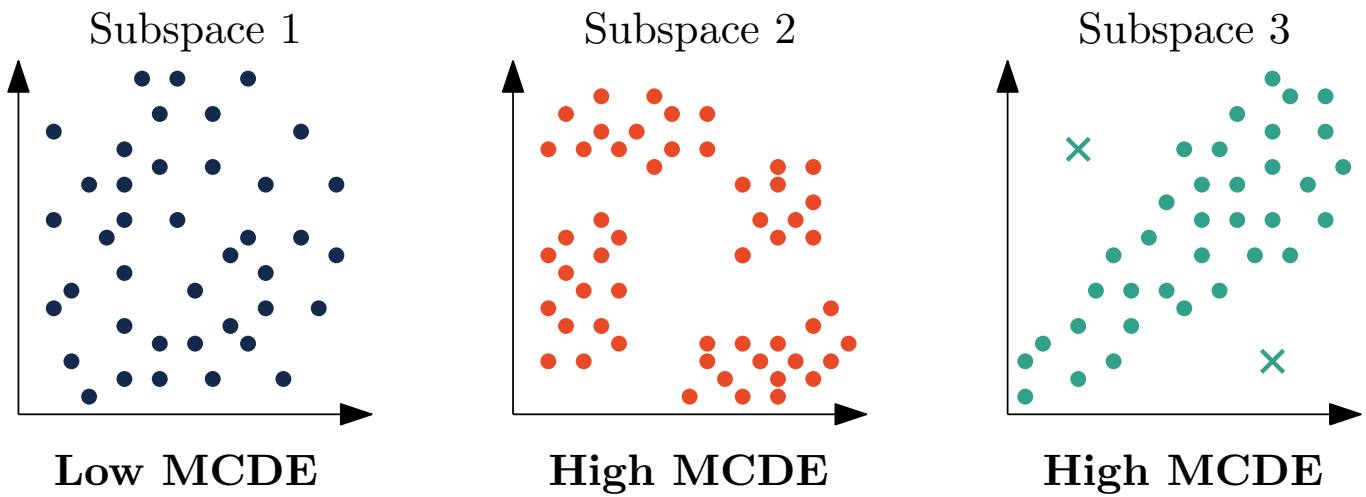

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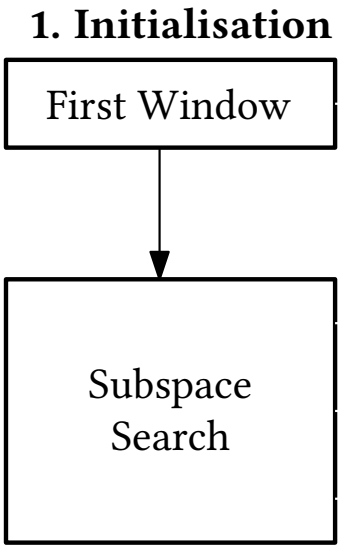

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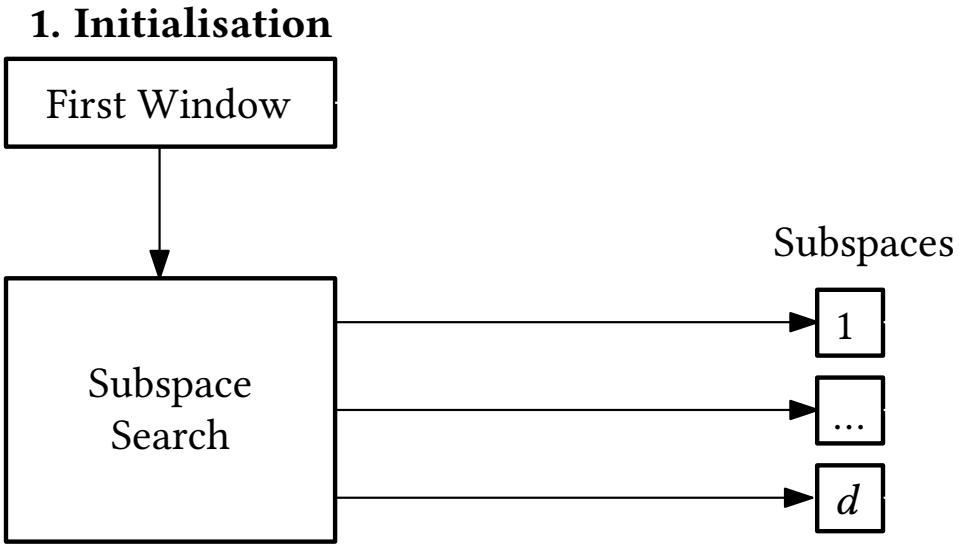

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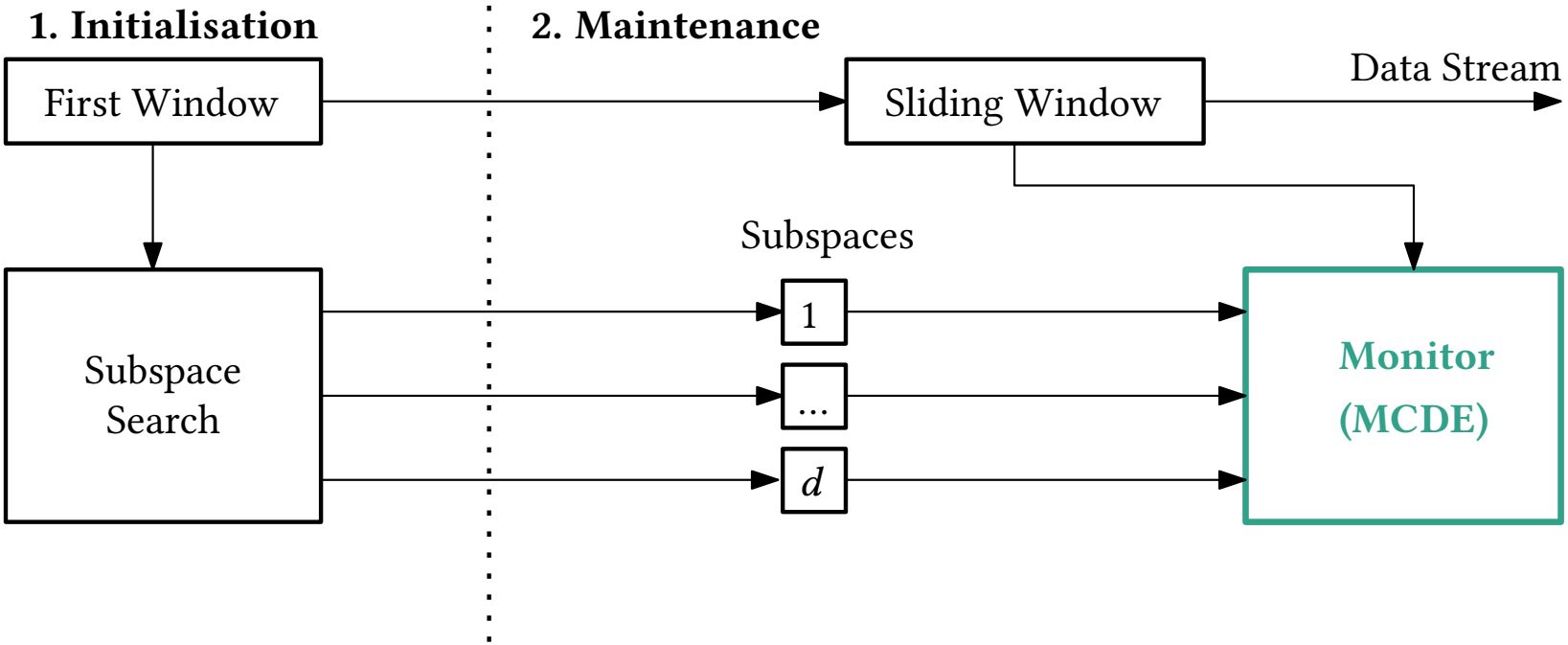

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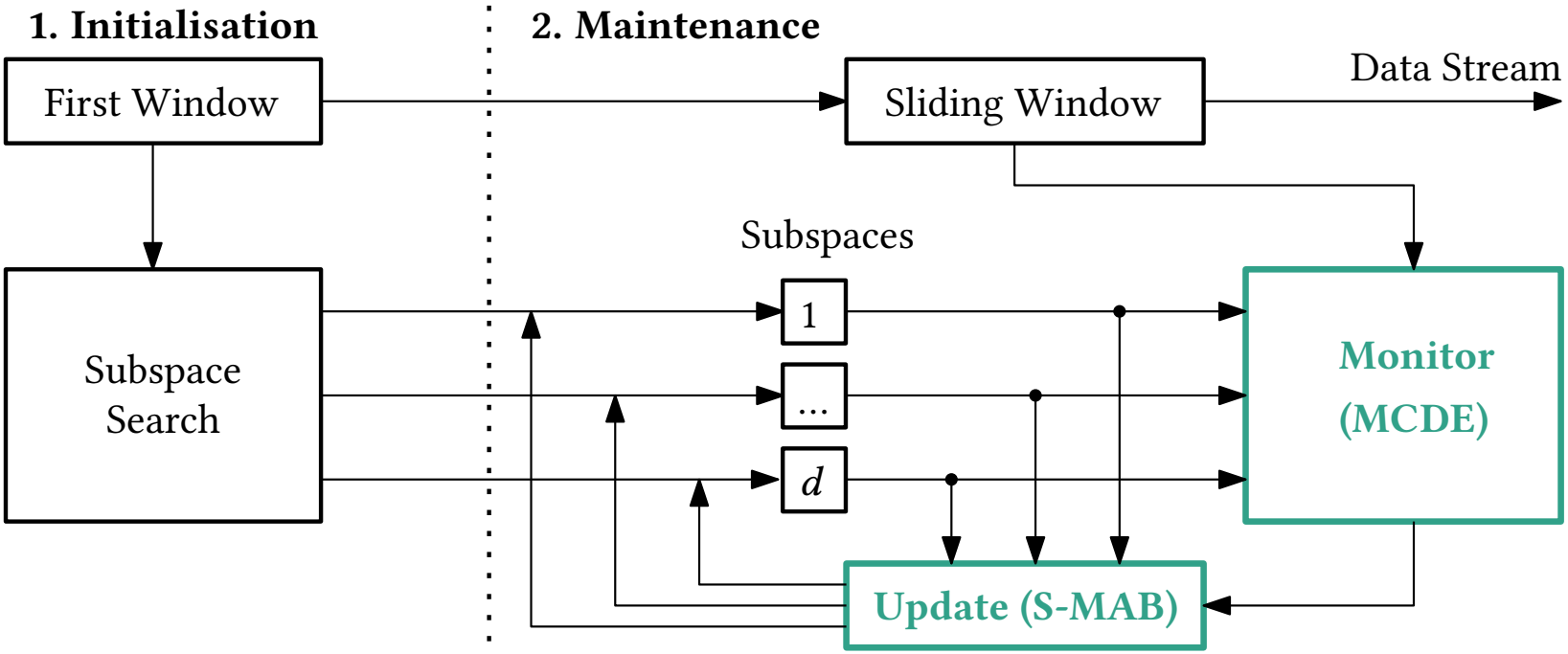

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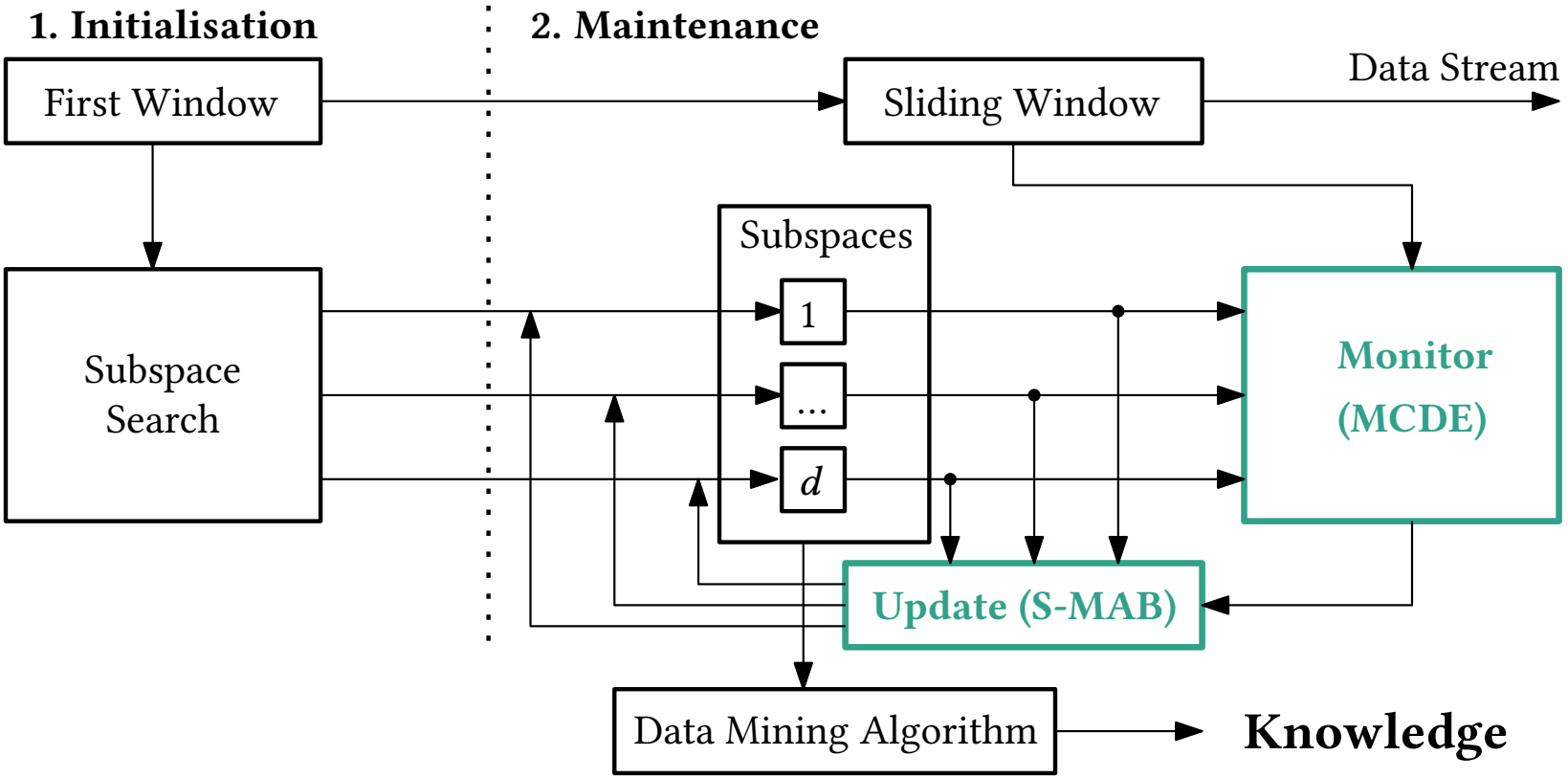

SGMRD improves Outlier Detection

- We use the subspaces to build an “ensemble” outlier detector.
- We find that our method outperform state-of-the-art detectors.

Benchmark	Approach	AUC	AvgPrc	Prc@1%	Prc@2%	Prc@5%	Rcl@1%	Rcl@2%	Rcl@5%
ACTIVITY	**SGMRD**	**97.32**	**85.39**	**94.59**	**94.83**	**94.24**	**9.44**	**18.97**	**47.10**
	LOF	93.93	61.80	74.32	64.72	64.03	7.42	12.94	32.00
	STREAMHICS	88.52	47.38	70.72	54.61	51.89	7.06	10.92	25.93
	RS-STREAM	95.95	68.23	71.62	72.58	75.00	7.15	14.52	37.48
	XSTREAM	77.71	20.41	3.60	10.14	16.31	0.36	2.02	8.13
KDDCUP99	**SGMRD**	**69.98**	**10.29**	**0.00**	**0.20**	**0.56**	**0.00**	**0.06**	**0.39**
	LOF	65.07	9.57	0.00	0.00	0.08	0.00	0.00	0.06
	STREAMHICS	57.11	7.89	0.00	0.00	0.08	0.00	0.00	0.06
	RS-STREAM	43.21	5.73	0.00	0.00	0.08	0.00	0.00	0.06
	XSTREAM	52.70	8.23	0.00	0.20	0.08	0.00	0.06	0.06
SYNTH50	**SGMRD**	**75.87**	**31.27**	**27.00**	**16.00**	**7.60**	**33.33**	**39.51**	**46.91**
	LOF	61.38	1.08	0.00	0.50	0.60	0.00	1.23	3.70
	STREAMHICS	63.90	12.00	11.00	6.00	3.40	13.58	14.81	20.99
	RS-STREAM	46.52	0.73	0.00	0.00	0.00	0.00	0.00	0.00
	XSTREAM	48.43	0.90	1.00	0.50	1.40	1.23	1.23	8.64

SGMRD improves Outlier Detection

- We use the subspaces to build an “ensemble” outlier detector.
- We find that our method outperform state-of-the-art detectors.

Benchmark	Approach	AUC	AvgPrc	Prc@1%	Prc@2%	Prc@5%	Rcl@1%	Rcl@2%	Rcl@5%
ACTIVITY	**SGMRD**	**97.32**	**85.39**	**94.59**	**94.83**	**94.24**	**9.44**	**18.97**	**47.10**
	LOF	93.93	61.80	74.32	64.72	64.03	7.42	12.94	32.00
	STREAMHICS	88.52	47.38	70.72	54.61	51.89	7.06	10.92	25.93
	RS-STREAM	95.95	68.23	71.62	72.58	75.00	7.15	14.52	37.48
	XSTREAM	77.71	20.41	3.60	10.14	16.31	0.36	2.02	8.13
KDDCUP99	**SGMRD**	**69.98**	**10.29**	**0.00**	**0.20**	**0.56**	**0.00**	**0.06**	**0.39**
	LOF	65.07	9.57	0.00	0.00	0.08	0.00	0.00	0.06
	STREAMHICS	57.11	7.89	0.00	0.00	0.08	0.00	0.00	0.06
	RS-STREAM	43.21	5.73	0.00	0.00	0.08	0.00	0.00	0.06
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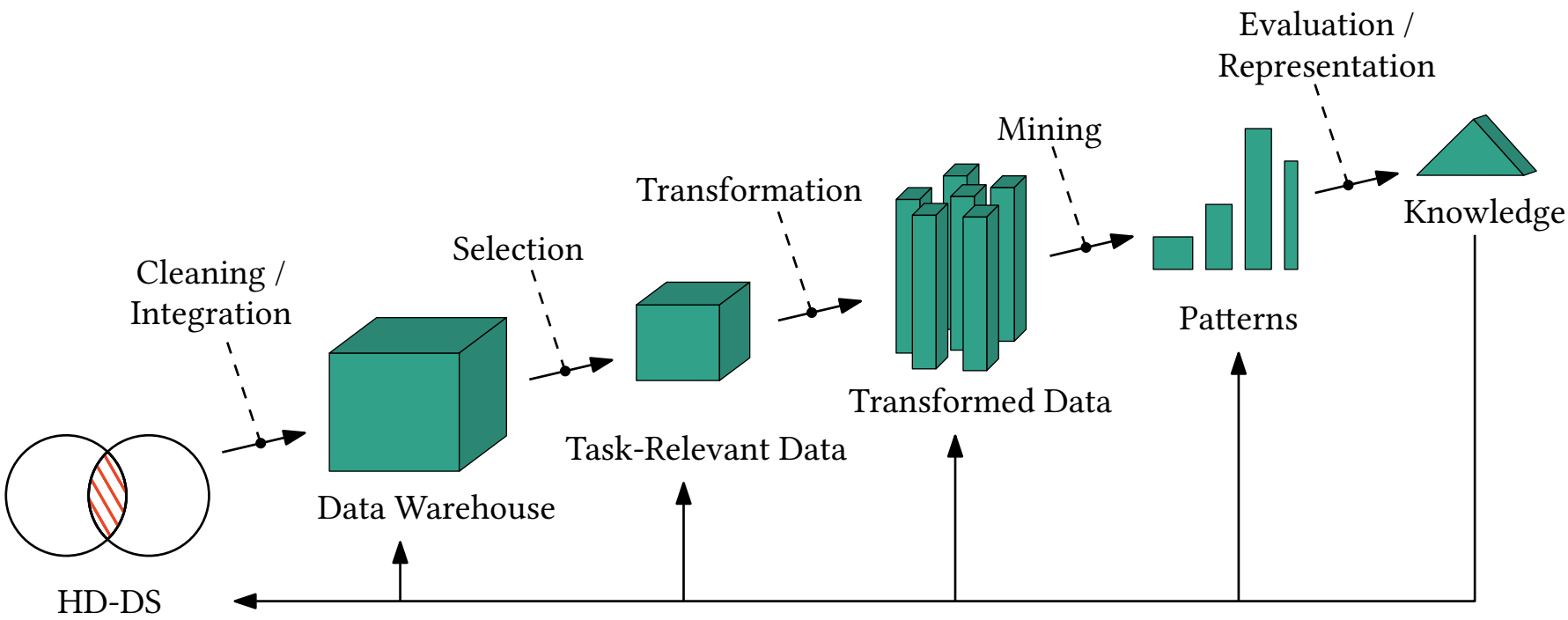
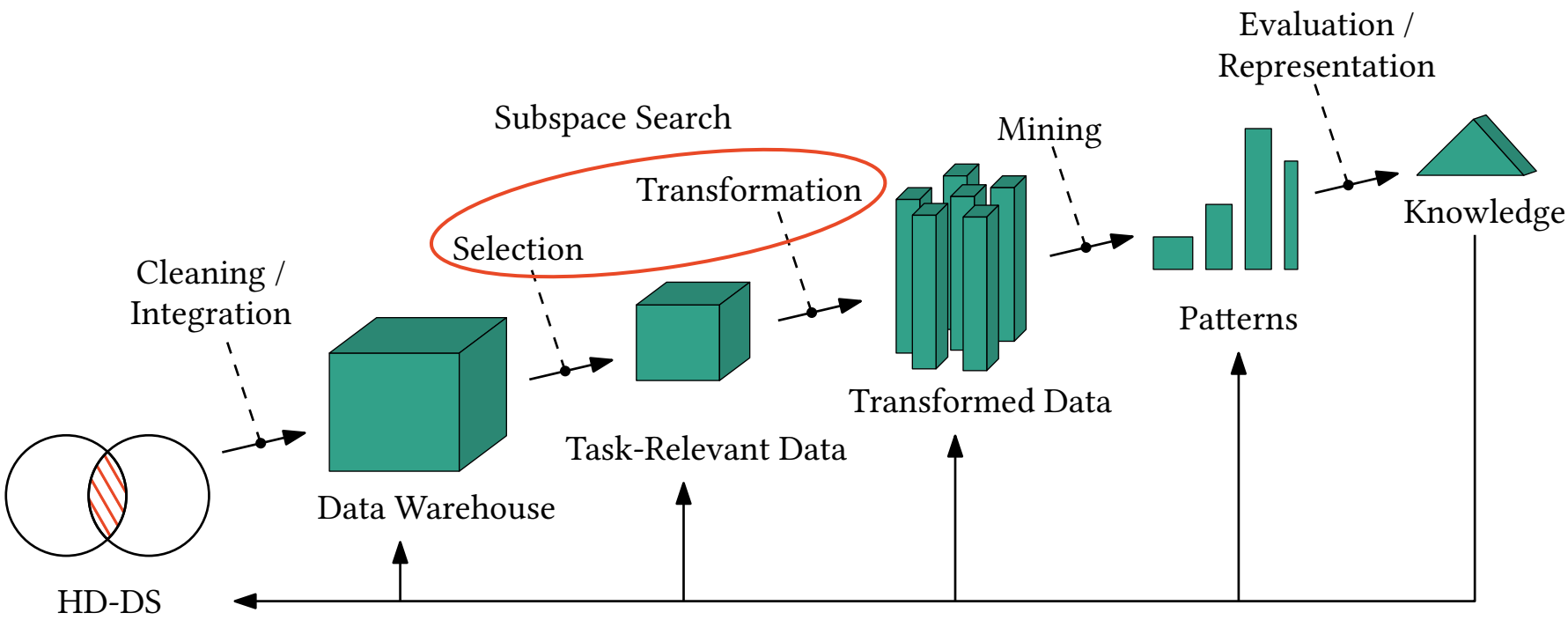
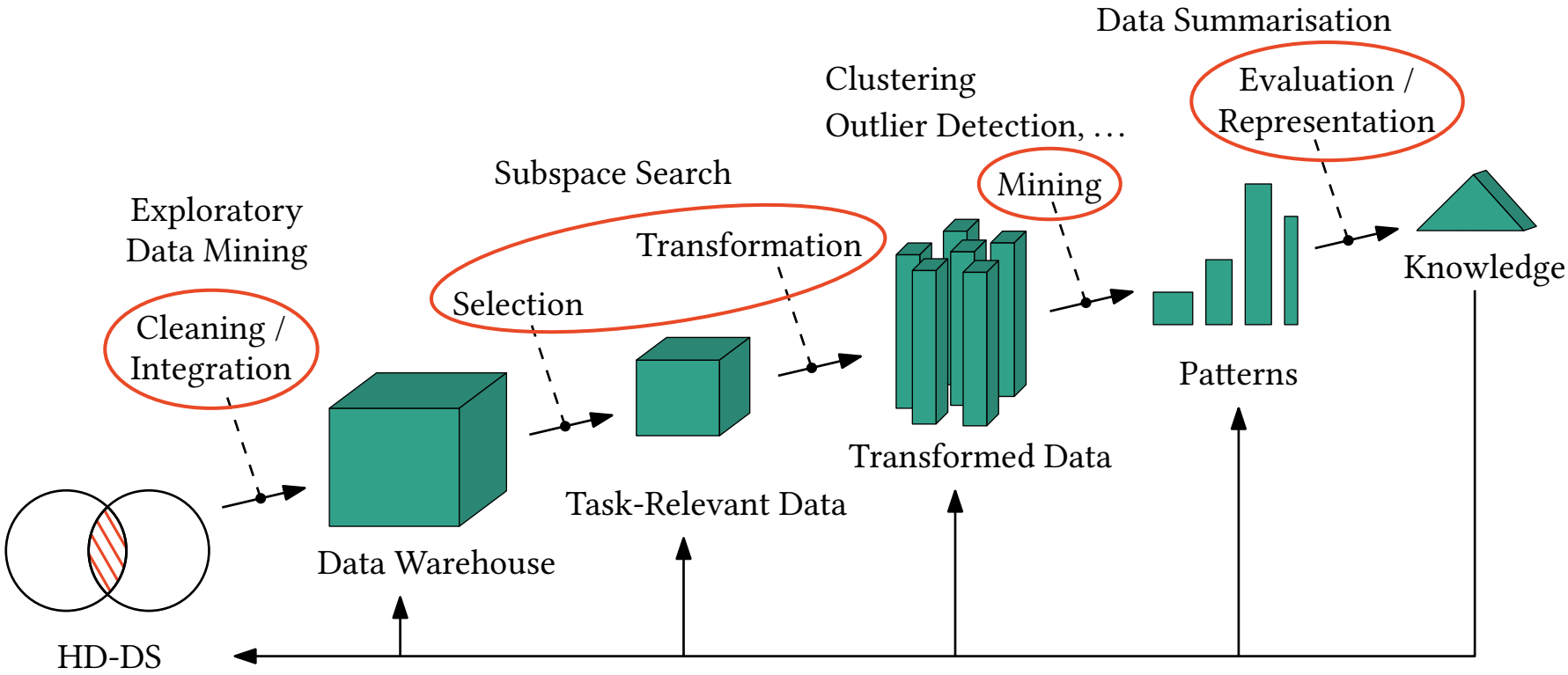
Addressing KDD in HD-DS



Addressing KDD in HD-DS



Addressing KDD in HD-DS



Conclusion

With our contributions, we can now **estimate** and **monitor dependency** in **high-dimensional data streams**, which facilitates **knowledge discovery** in this challenging, real-world setting.

- **Estimating Dependency:** MCDE [FB19] [FMKB20]
- **Monitoring:** S-MAB [FKB19]
- **Knowledge Discovery:** SGMRD [FKB20], kj-NN [FMG+20]
- Reproducibility: `https://github.com/edouardfouche`

Thanks to everyone who made this possible!

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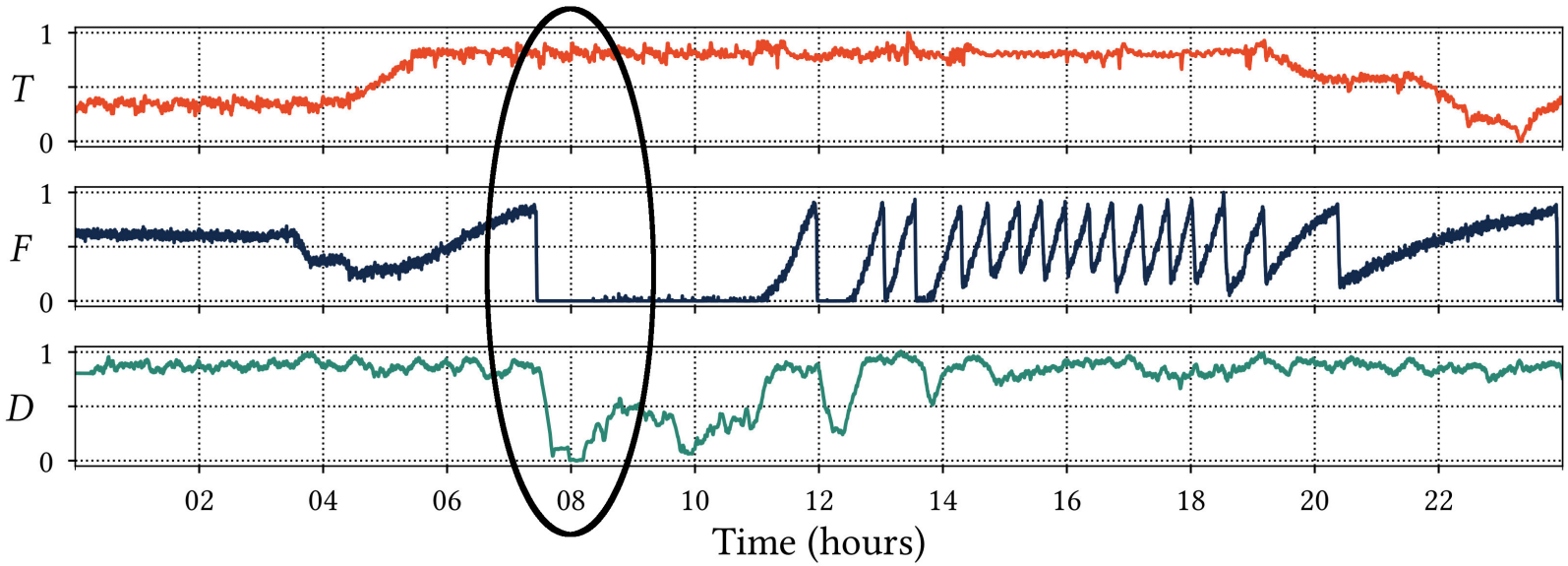
Dependency helps to identify patterns

An example with two streams:

- T: Temperature in the reactor
- F: Filling level of the cyclone
- D: Estimation of dependency between T and F



$\rightarrow$ Monitoring Dependency shows interruption in production

Benchmarking Dependency Estimation

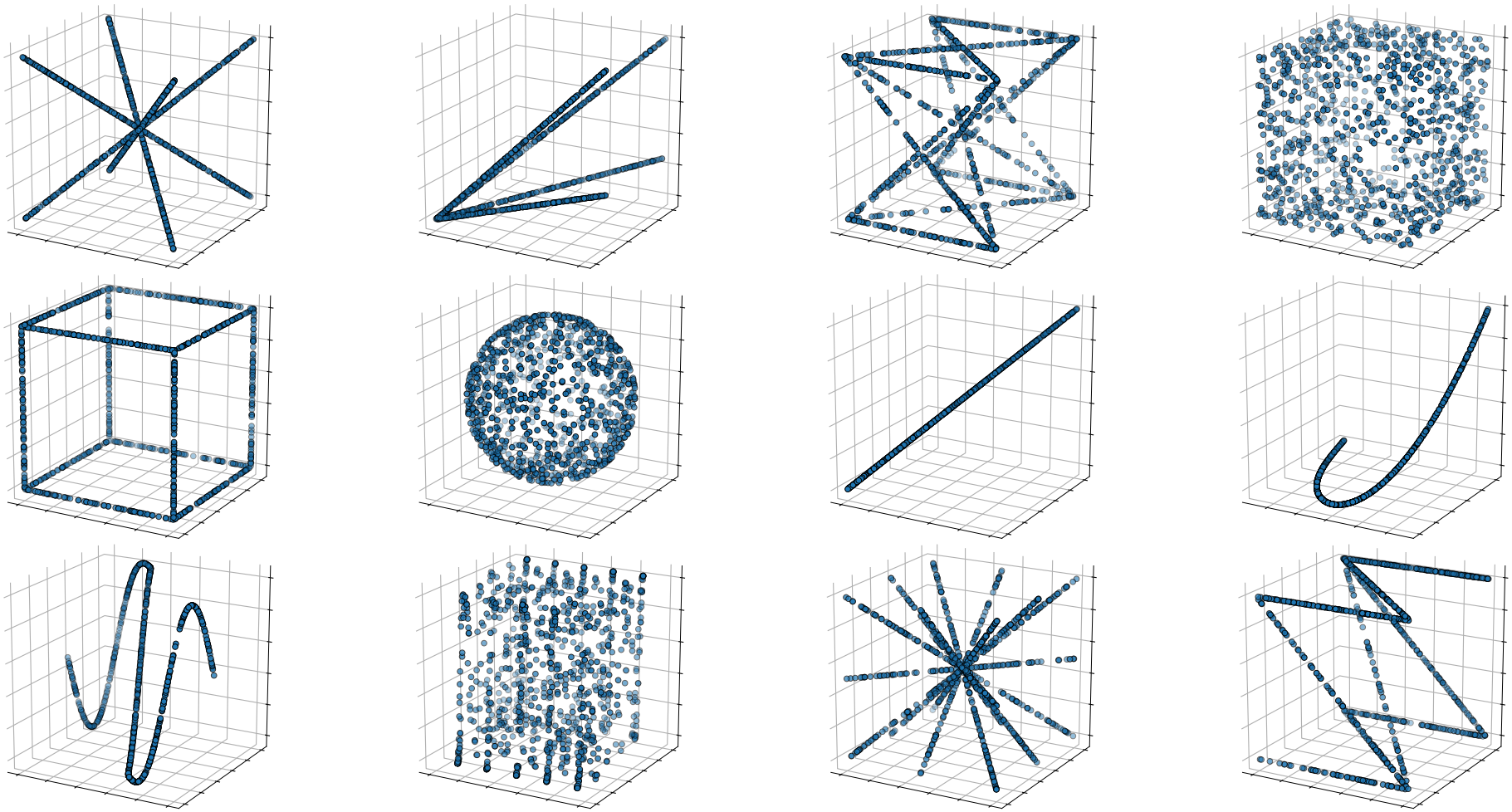
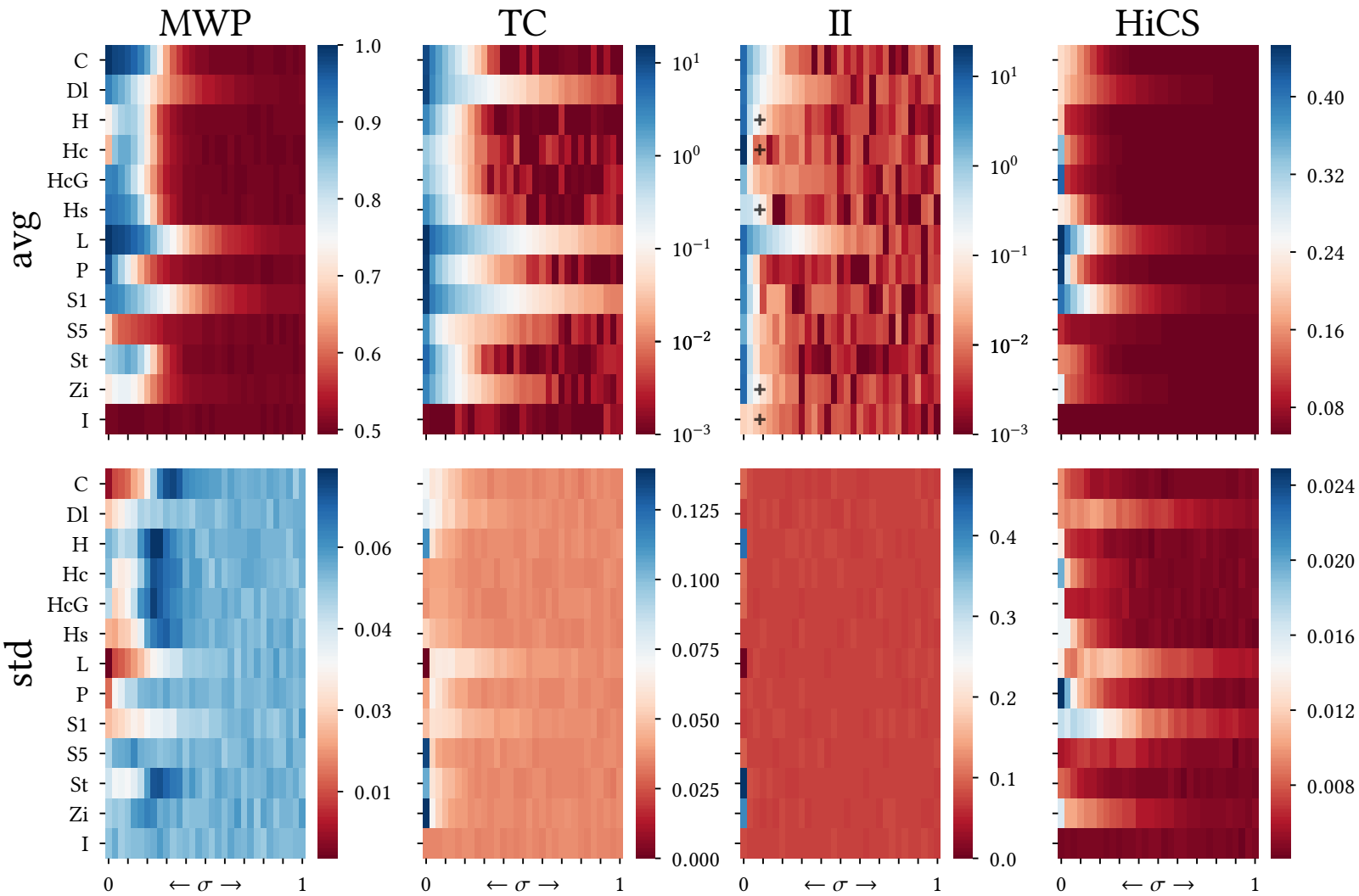
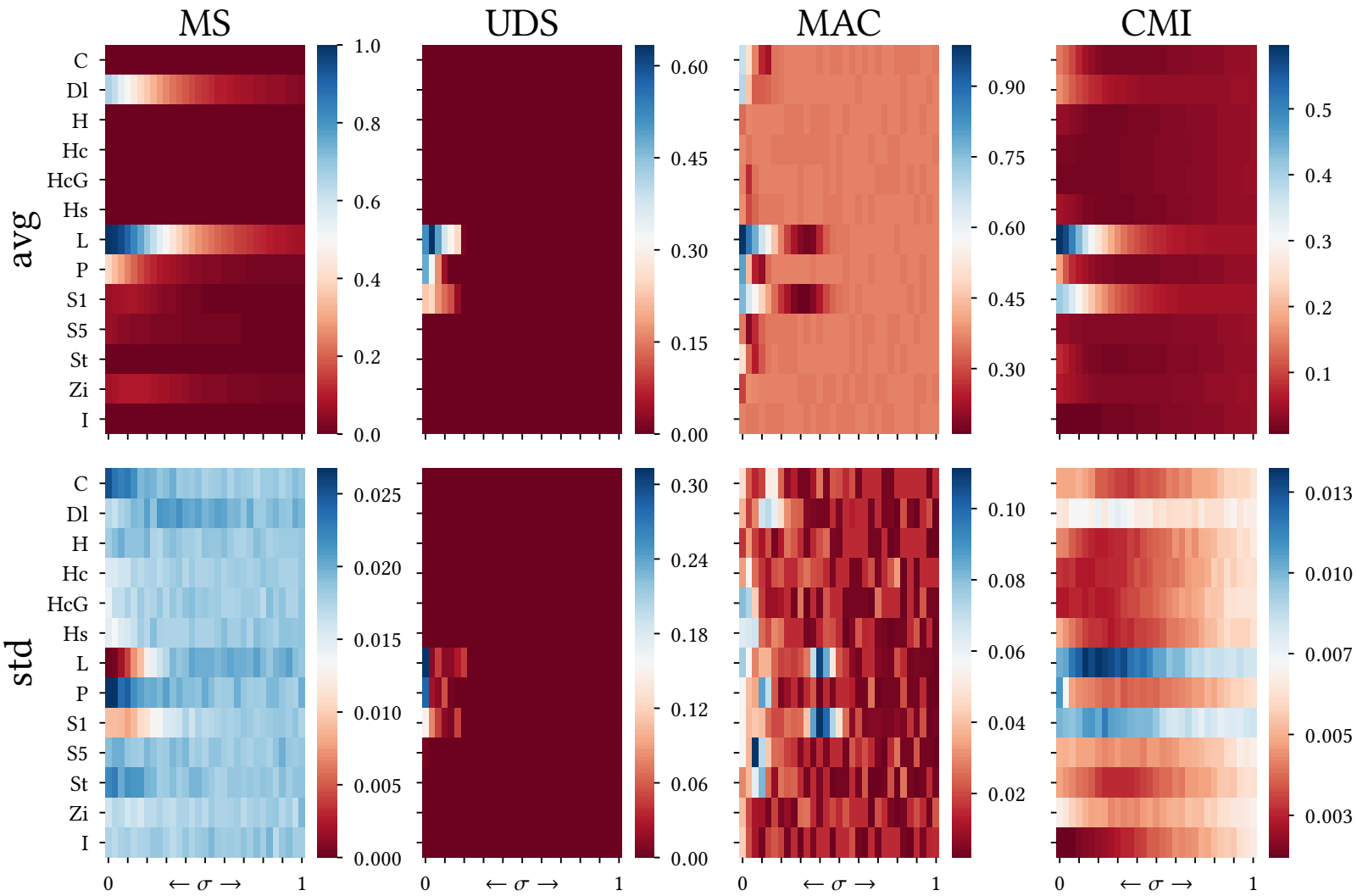


Figure 2: An assortment of 12 dependencies

Statistical Power of MCDE



Statistical Power of MCDE



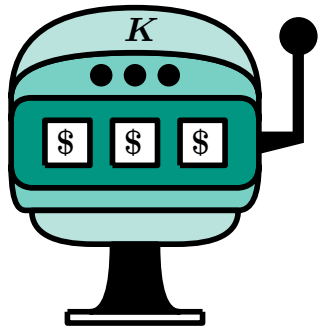
The “Classical” MAB

Let there be a set of K arms, $[K] = \{1, \ldots, K\}$.

The rewards of each arm $i \in [K]$ follow a Bernoulli distribution $\mathcal{B}_i$ with mean μ_i.

At each round $t = 1, \ldots, T$:

- The forecaster chooses **one** arm $i \in [K]$
- Then, they observe a reward $X_t \sim \mathcal{B}_i$
- They update their estimation $\hat{\mu}_i$ of μ_i



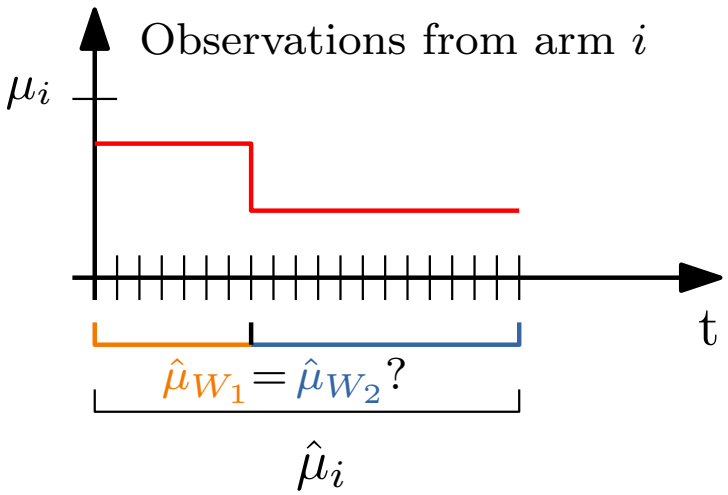
The goal of the forecaster is to maximize their gain, i.e., $\sum_{t=1}^{T} X_t$

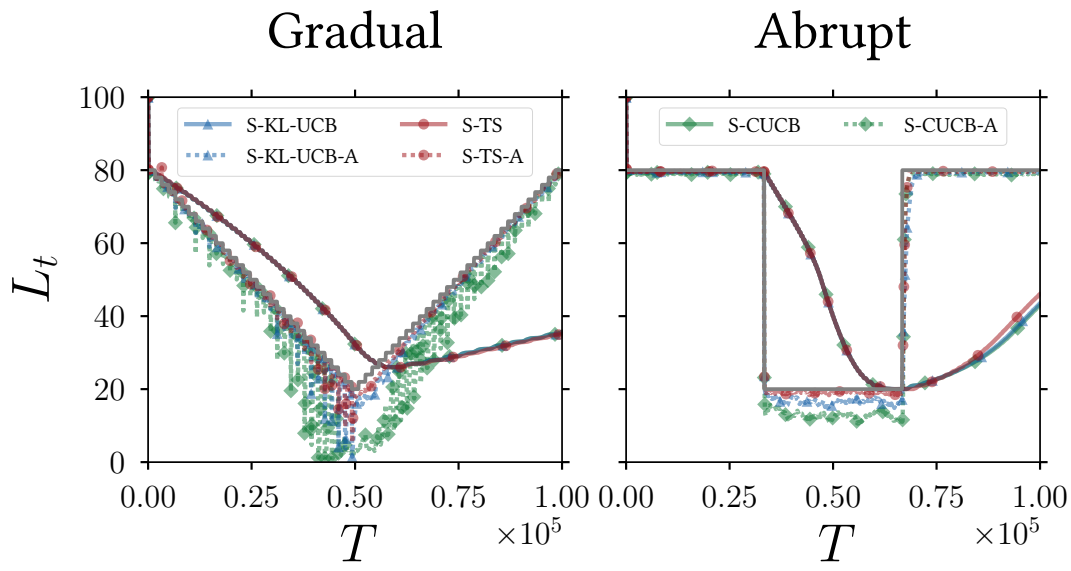
S-MAB with ADWIN

Problem: The expectations μ_i of each arm $i \in [K]$ might change.

We use Adaptive Windowing (ADWIN) [BG07]

- Maintain $\hat{\mu}_i$ for each arm over a sliding window of adaptive length





→ Scaling Thompson Sampling with ADWIN (S-TS-A)

Deploying S-MAB @ Bioliq

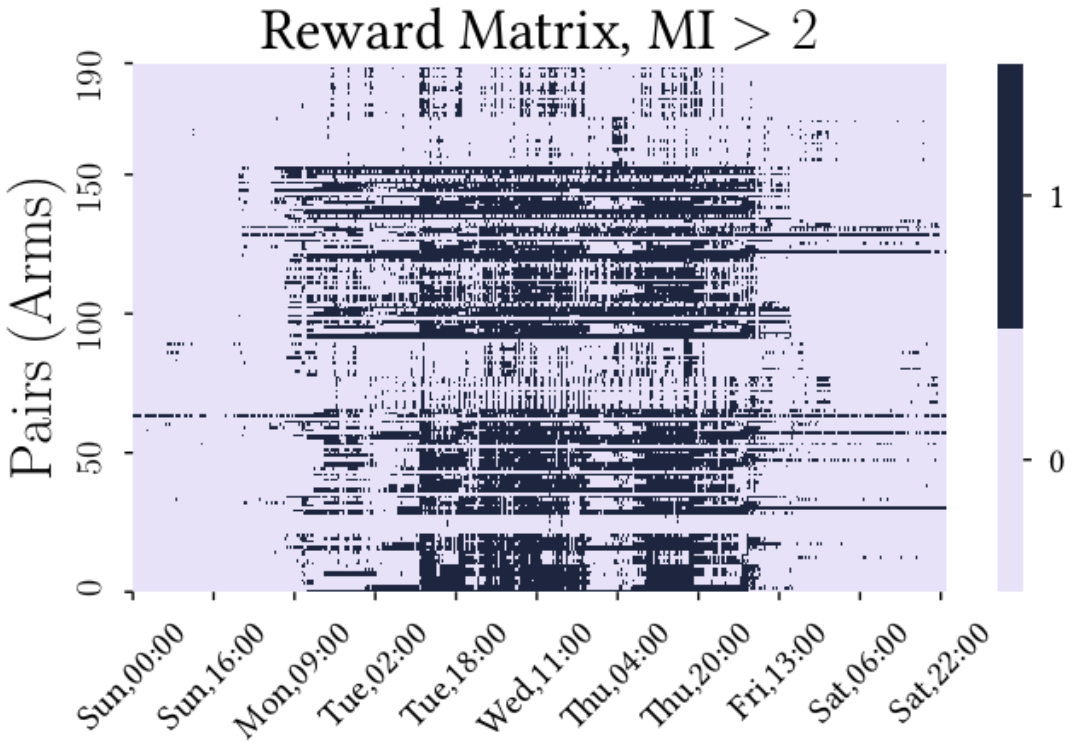
Bioliq: 20 sensors, 1 week data

- Mutual Information (MI) over sliding window
  - Window Size: 1000 points ($\sim$ 15 minutes)
  - Step size: 100 points

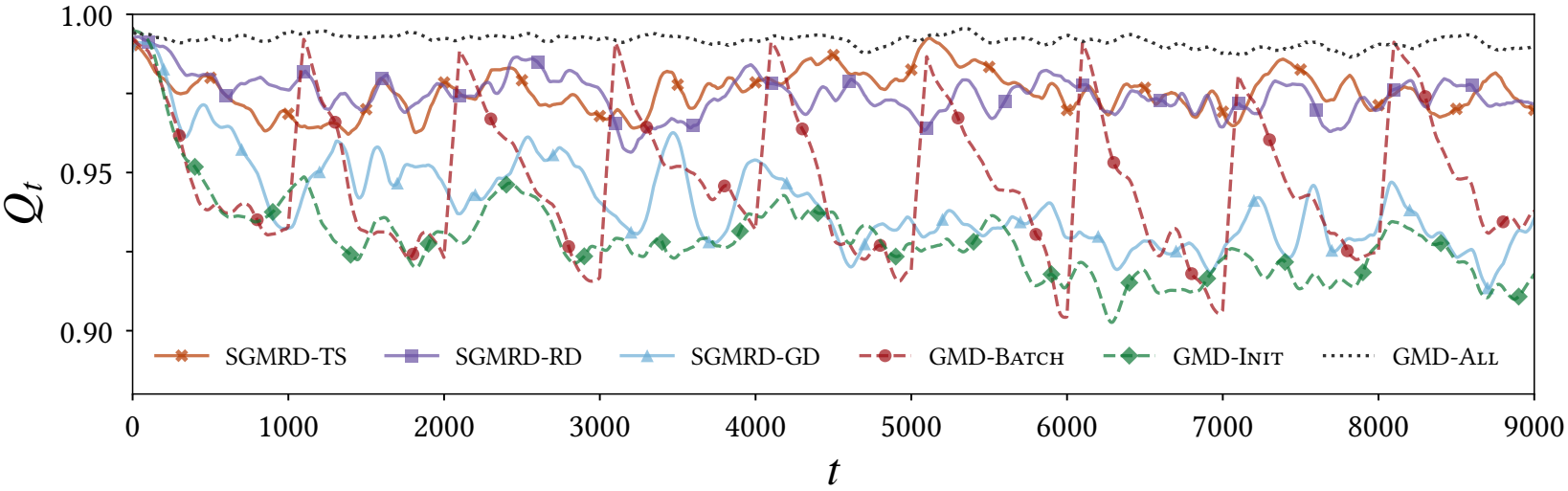
S-MAB as a "monitoring system"

- If MI ≥ 2, Reward $= 1$

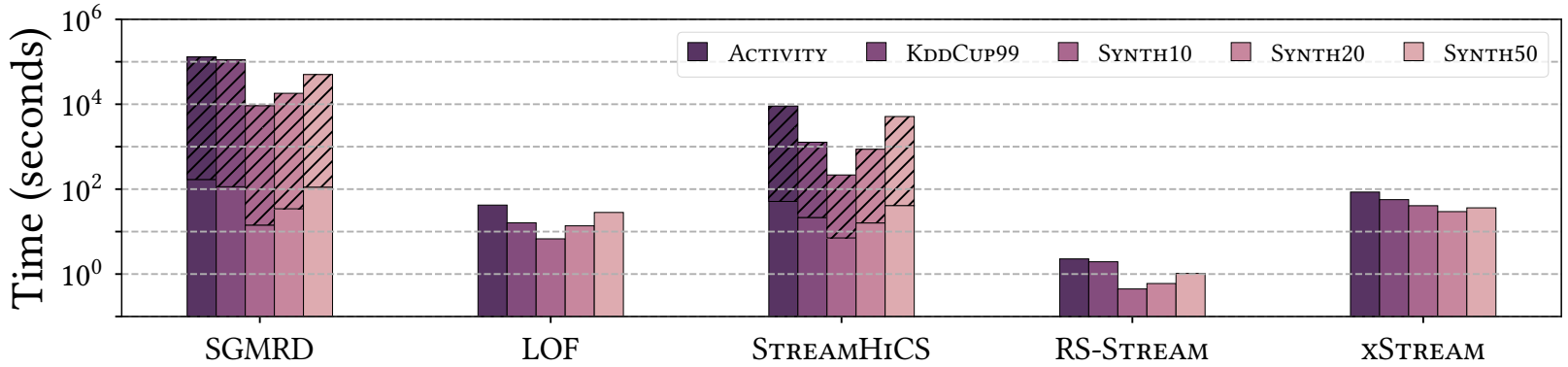
The environment is non-static !



SGMRD: Subspace Monitoring

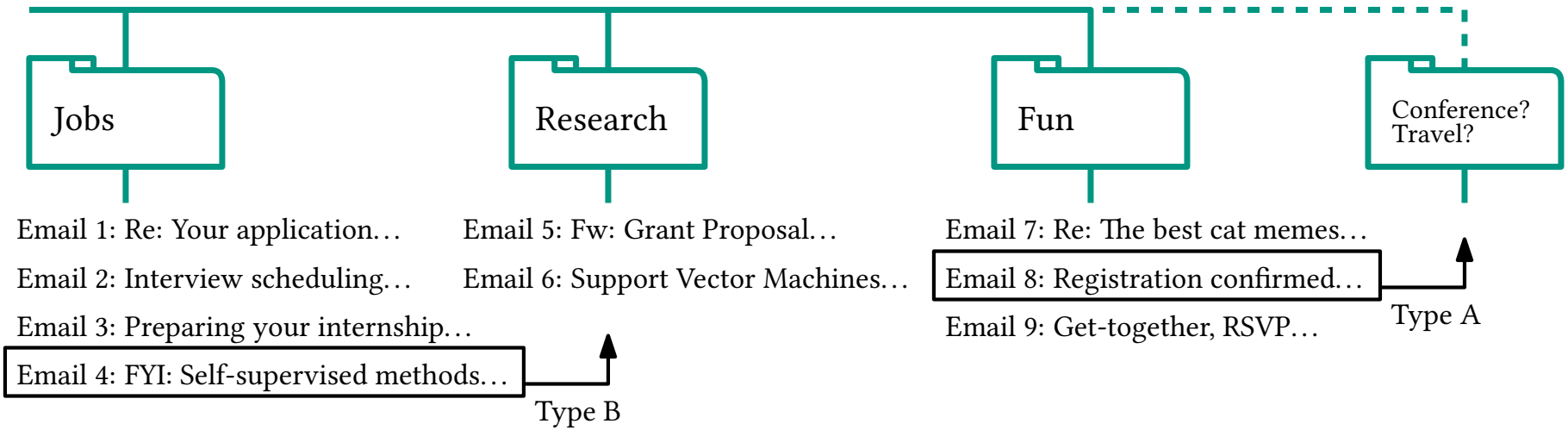


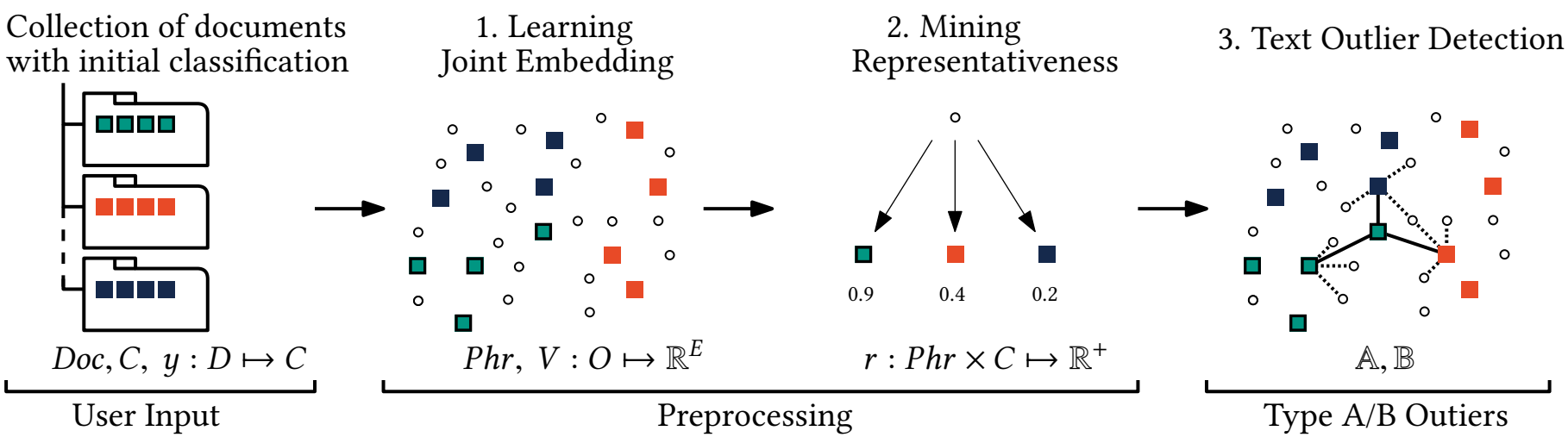
Average quality of monitored subspaces



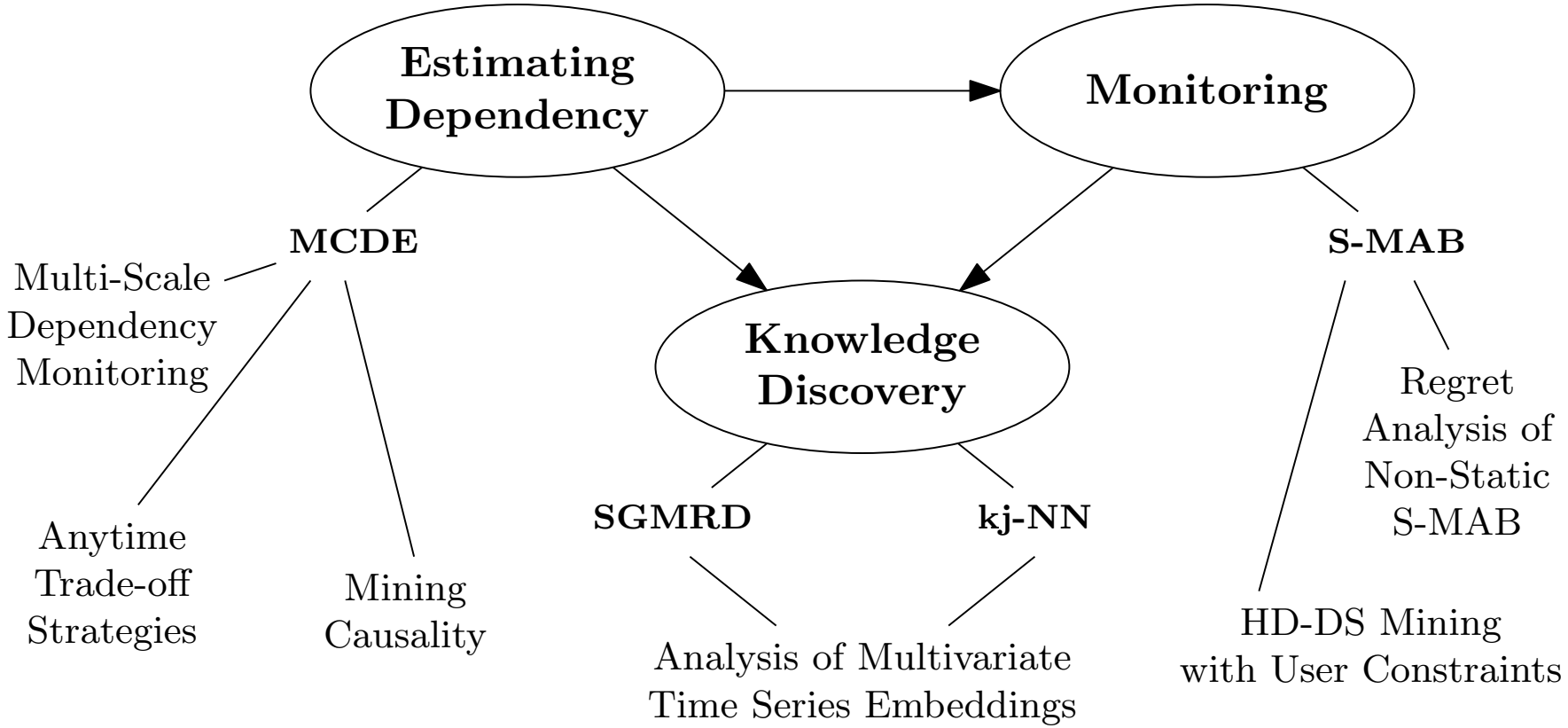
Outlier detection runtime

Text Outlier Detection (kj-NN)





Outlook


Estimating Dependency
Monitoring
MCDE
S-MAB
Multi-Scale Dependency Monitoring
Knowledge Discovery
Regret Analysis of Non-Static S-MAB
Anytime Trade-off Strategies
Mining Causality
SGMRD
kj-NN
HD-DS Mining with User Constraints
Analysis of Multivariate Time Series Embeddings

Mining Causality

- Dependencies may be spurious
  - e.g., see Simpson's paradox
- With MCDE, we may detect such spurious relationships.
  - Build a "dependency network"
  - In HD-DS