DiffPrep: Differentiable Data Preprocessing Pipeline Search for Learning over Tabular Data

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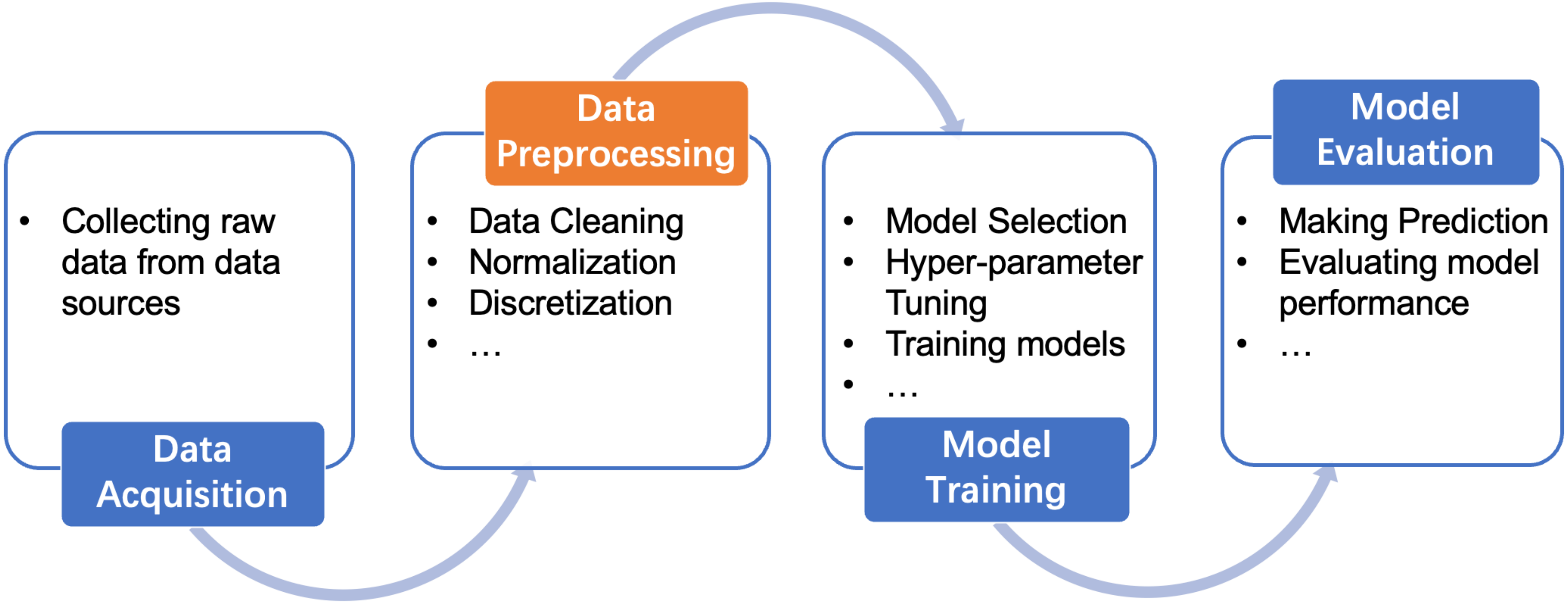
Data preprocessing is an essential step in ML

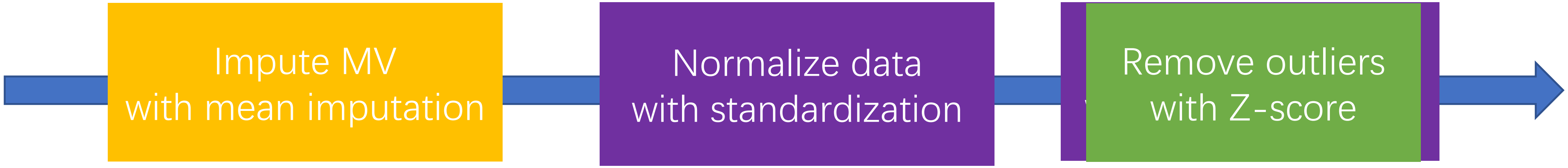
- Raw data collected from data sources can rarely be used directly by ML models due to the existence of data issues (e.g., data errors, different feature scales).



A Typical ML Workflow

Designing a data preprocessing pipeline is hard

- **Data Preprocessing Pipeline** is a sequence of operators, where each operator tackles one specific data issue.



An example data preprocessing pipeline

- **Complex design decisions:**
  - **Types:** which type of transformations to use?
  - **Operators:** which operator to use for each transformation?
  - **Order:** which order of transformations to use?
  - **Feature-wise:** different features may need different pipelines.

Limitations in Existing Methods

- **ML Developers**
  - Use a default pipeline or trial-and-error methods.
- **Traditional Data Cleaning Work**
  - Design pipelines that optimize data quality independently of ML.
  - Data quality may not be accessible, and it may not lead to the optimal ML performance.
- **Existing AutoML Systems**
  - Limited search space.
  - Train model multiple times.

Systems	Operator	Types	Order	Feature-wise	Optimization Method
H2O	×	×	×	×	Random Search
Azure	✓	×	×	×	Bayesian Optimization
Auto-Sklearn	✓	✓	×	×	Bayesian Optimization
Learn2Clean	✓	✓	✓	×	Q-Learning
DiffPrep-Fix	✓	✓	×	✓	**Bi-level Optimization with Gradient Descent**
DiffPrep-Flex	✓	✓	✓	✓	

Problem Definition

- **Goal:** automatically and efficiently select a data preprocessing pipeline from the search space such that the model performance (validation accuracy) is maximized.

Outer level: $$\underset{pipline}{\operatorname{argmin}} Loss\ (D_{val}, pipeline, model^*)$$

Inner level: $$s.t.\ model^* = \underset{model}{\operatorname{argmin}} Loss\ (D_{train}, pipeline, model)$$

"Bi-level Optimization"

- **Compared with existing AutoML systems:**
  - Explore the entire design space of data preprocessing pipelines (types, operators, order, feature-wise).
  - Only need to train ML model once.

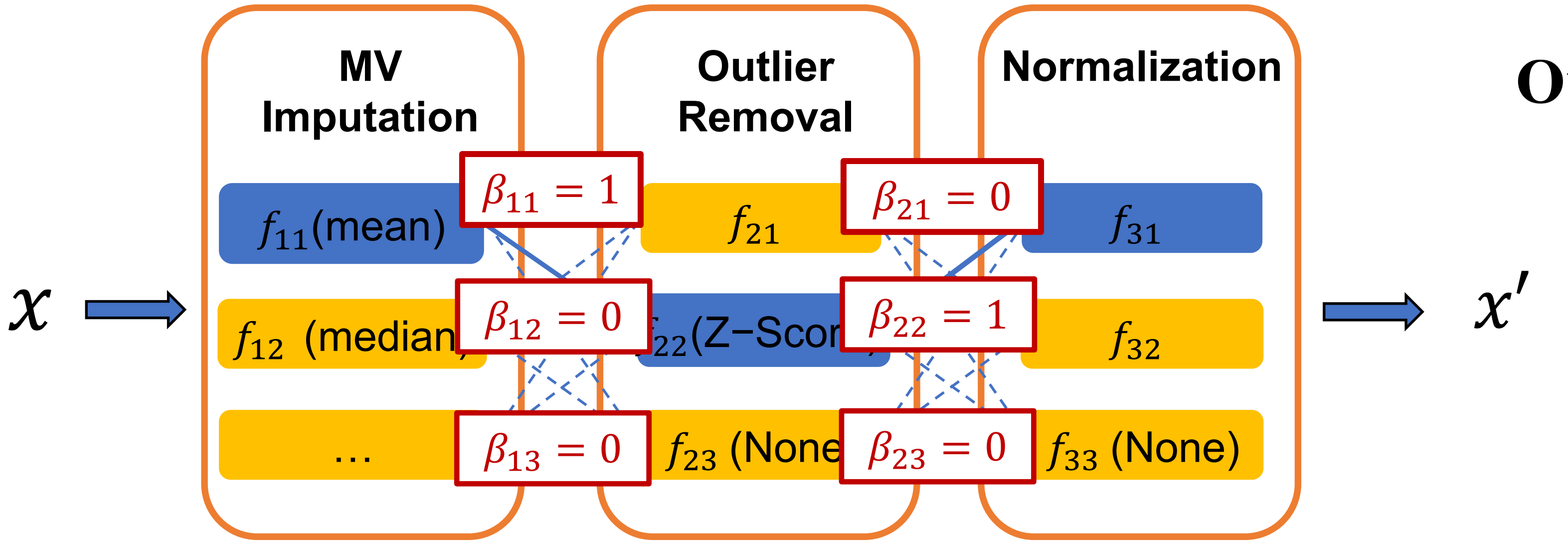
Gradient-based Bi-level Optimization

- **Naive Approach:** we train a ML model with every possible pipeline and select the best one. --- Assume a pipeline contains s transformations and m choices for each transformation. There are m^{sc} feature-wise pipelines for a dataset with c features.
- **Gradient-based approach:** we alternatively and iteratively solve the outer-level and inner-level optimization using gradient descent.
- **Key issue:** the search space of pipelines is discrete and non-differentiable.

Can we convert the discrete search space into a ***continuous and differentiable*** space?

Step 1: Parameterization

- **Goal:** Represent each pipeline in the space using a set of parameters
- Let's first assume we have a predefined order of transformations.



Output of a transformation:

$$x_i = \sum_j \beta_{ij} f_{ij}(x_{i-1})$$

Output of pipeline:

$$x'(x, \boldsymbol{\beta})$$

Loss:

$$Loss\ (D_{val}, \boldsymbol{\beta}, \boldsymbol{w})$$

$$Loss\ (D_{train}, \boldsymbol{\beta}, \boldsymbol{w})$$

Associate each operator with a $\beta_{ij} \in \{0,1\}$

$$\beta_{ij} = \begin{cases} 1 & f_{ij} \text{ is selected} \\ 0 & \text{Otherwise} \end{cases}$$

Constraint: $\sum_j \beta_{ij} = 1$

Step 2: Relaxation

$\boldsymbol{\beta}: \beta_{ij} \in \{0,1\} \xrightarrow{\text{Relax}} \boldsymbol{\beta}: \beta_{ij} \in [0,1]$

- To retain constraints $\sum_j \beta_{ij} = 1$, use **Softmax function**, $\tau_{ij} \in \mathbb{R}$

$$\beta_{ij} = \frac{\exp(\tau_{ij})}{\sum_k \exp(\tau_{ik})}$$

We can now solve Bi-level optimization using gradient descent

Automate Order Selection

- **Question:** How to determine the order of applying transformations (e.g., Outlier Removal, Discretization, Normalization)?
  - Can we try all possible orders? --- The number of possible orders for feature-wise pipelines are exponential to the number of features.

- **Parameterization**: Any order can be represented using a binary permutation matrix α

$$\alpha_{ij} = \begin{cases} 1 & \text{the i-th type is } F_j \\ 0 & \text{Otherwise} \end{cases}$$

$$[\mathrm{O}, \mathrm{D}, \mathrm{N}] \longrightarrow \boldsymbol{\alpha} = \begin{array}{c} \begin{array}{ccc} \mathrm{N} & \mathrm{O} & \mathrm{D} \end{array} \\ \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \end{array}$$

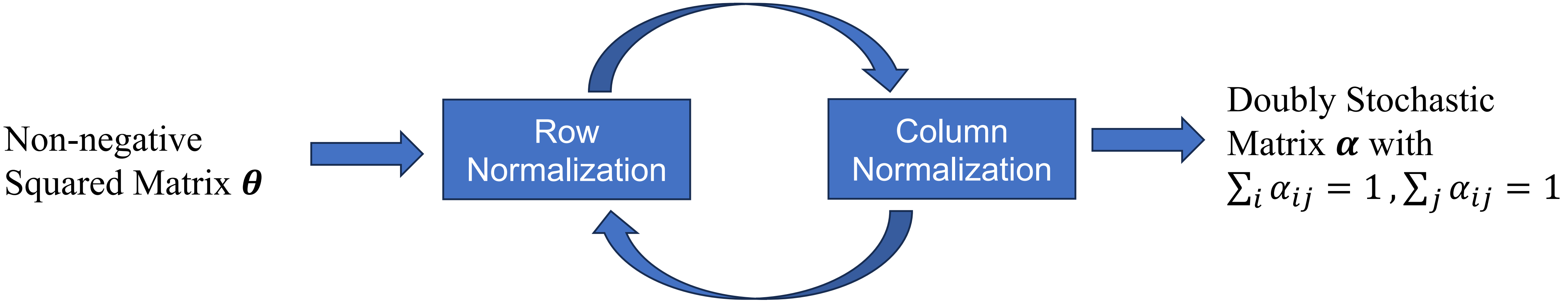
Constraints: $\sum_i \alpha_{ij} = 1 , \sum_j \alpha_{ij} = 1$

Automate Order Selection

- **Relaxation:**

$$\boldsymbol{\alpha}: \alpha_{ij} \in \{0,1\} \xrightarrow{\text{Relax}} \boldsymbol{\alpha}: \alpha_{ij} \in [0,1]$$

To retain constraints $\sum_i \alpha_{ij} = 1\,, \sum_j \alpha_{ij} = 1$, use *Sinkhorn normalization*



We can now learn optimal order, choices of operators and the model simultaneously!

Experiment Setup

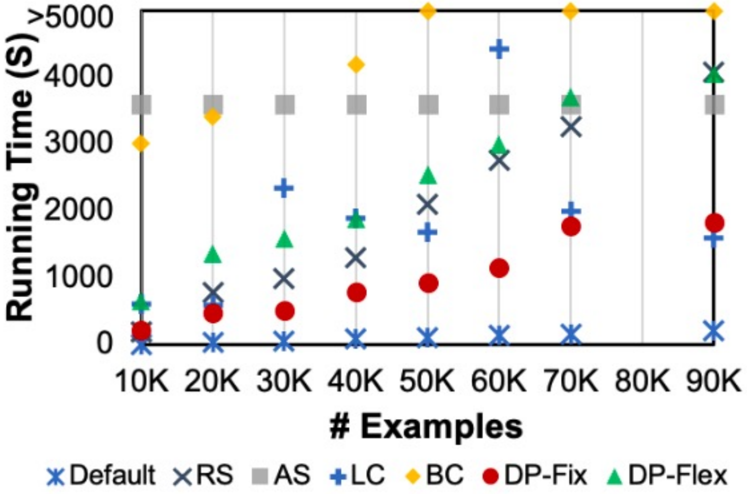
- **Datasets:** 18 real-world datasets
- **Model:** Logistic regression
- **Search Space:** Missing value imputation, Outlier removal, Discretization, Normalization
- **Methods compared:**

Our methods	Practical Methods	AutoML Systems	Advanced Data Cleaning Methods
DiffPrep-Fix (DP-Fix) DiffPrep-Flex (DP-Flex)	Default (DEF) Random Search (RS)	AutoSklearn (AS)	BoostClean (Clean) Learn2Clean (LC)

- **Evaluation Metrics:**
  - Model accuracy
  - Running time

Experiment Results

Dataset	Data Characteristics					Test Accuracy						
	#Ex.	#Feat.	#Cls.	#MVs	#Out.	DEF	RS	AS	LC	BC	DP-Fix	DP-Flex
abalone	4177	9	28	0	200	0.24	0.243	0.216	0.186	0.168	0.238	**0.255**
ada_prior	4562	15	2	88	423	0.848	0.844	0.853	0.816	0.848	**0.854**	0.846
avila	20867	11	12	0	4458	0.553	0.598	0.615	0.597	0.585	**0.638**	0.63
connect-4	67557	43	3	0	45873	0.659	0.671	0.667	0.658	0.69	**0.732**	0.701
eeg	14980	15	2	0	209	0.589	0.658	0.657	0.641	0.659	**0.678**	0.677
jungle_chess	44819	7	3	0	0	0.668	0.669	0.678	0.676	0.667	**0.682**	**0.682**
micro	20000	21	5	0	8122	0.564	0.579	0.584	0.582	0.561	0.586	**0.588**
mozilla4	15545	6	2	0	290	0.855	0.922	**0.931**	0.854	0.930	0.923	0.922
obesity	2111	17	7	0	25	0.775	0.841	0.737	0.723	0.652	0.893	**0.896**
page-blocks	5473	11	5	0	1011	0.942	0.959	**0.969**	0.92	0.951	0.957	0.967
pbcseq	1945	19	2	1445	99	0.71	0.73	0.712	0.704	0.72	0.725	**0.743**
pol	15000	49	2	0	8754	0.884	0.879	0.877	0.737	0.903	0.904	**0.919**
run_or_walk	88588	7	2	0	8548	0.719	0.829	0.851	0.728	0.835	0.907	**0.917**
shuttle	58000	10	7	0	5341	0.964	0.996	**0.998**	0.997	0.997	**0.998**	0.997
wall-robot-nav	5456	25	4	0	1871	0.697	0.872	0.869	0.69	0.9	0.898	**0.914**
google	9367	9	2	1639	109	0.586	0.627	**0.664**	0.549	0.616	0.645	0.641
house	1460	81	2	6965	617	0.928	0.938	**0.945**	0.812	0.928	0.932	**0.945**
uscensus	32561	15	2	4262	2812	0.848	0.840	0.851	0.786	0.848	**0.857**	0.852



Our methods achieve the best test accuracy on 15 out of 18 datasets!

Thank you!