Automating Feature Subspace Exploration via Multi-Agent Reinforcement Learning

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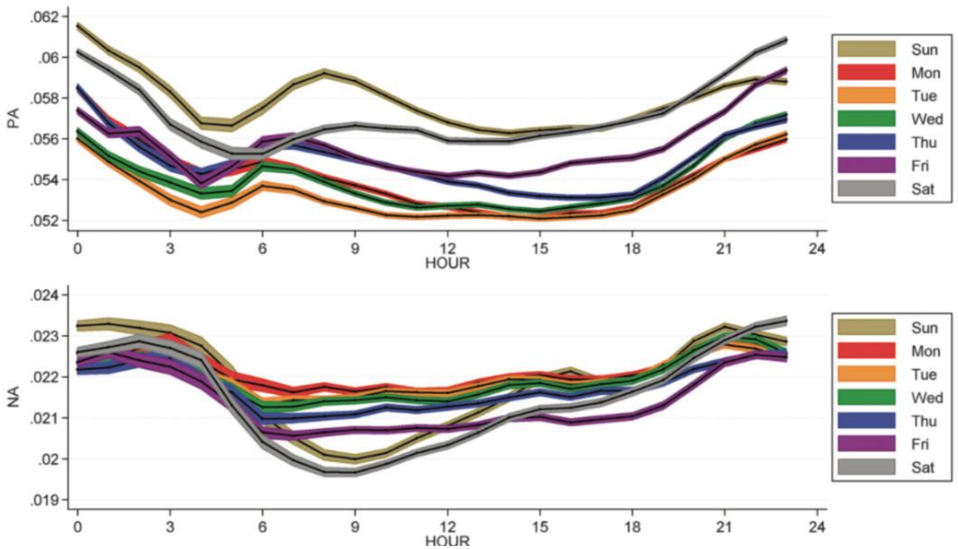
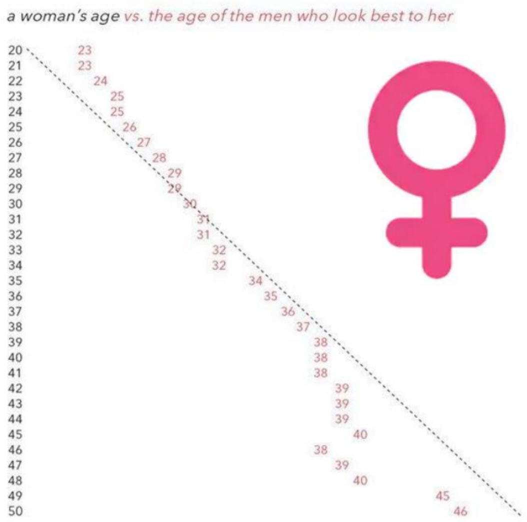
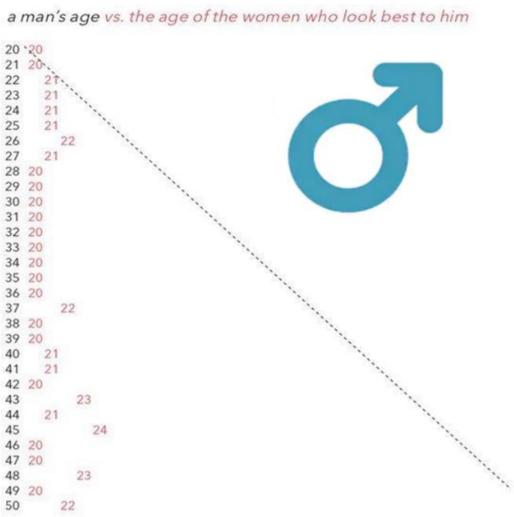
Background

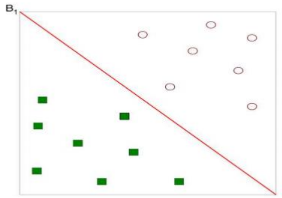
Feature Selection and Reinforcement Learning

Background





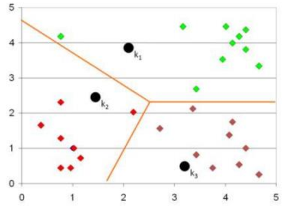




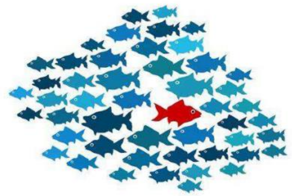
分类

TID	*Items*
1	Bread, Milk
2	Bread, Diaper, Beer, Eggs
3	Milk, Diaper, Beer, Coke
4	Bread, Milk, Diaper, Beer
5	Bread, Milk, Diaper, Coke

关联规则



聚类



离群检测

Feature Selection

What is feature selection?

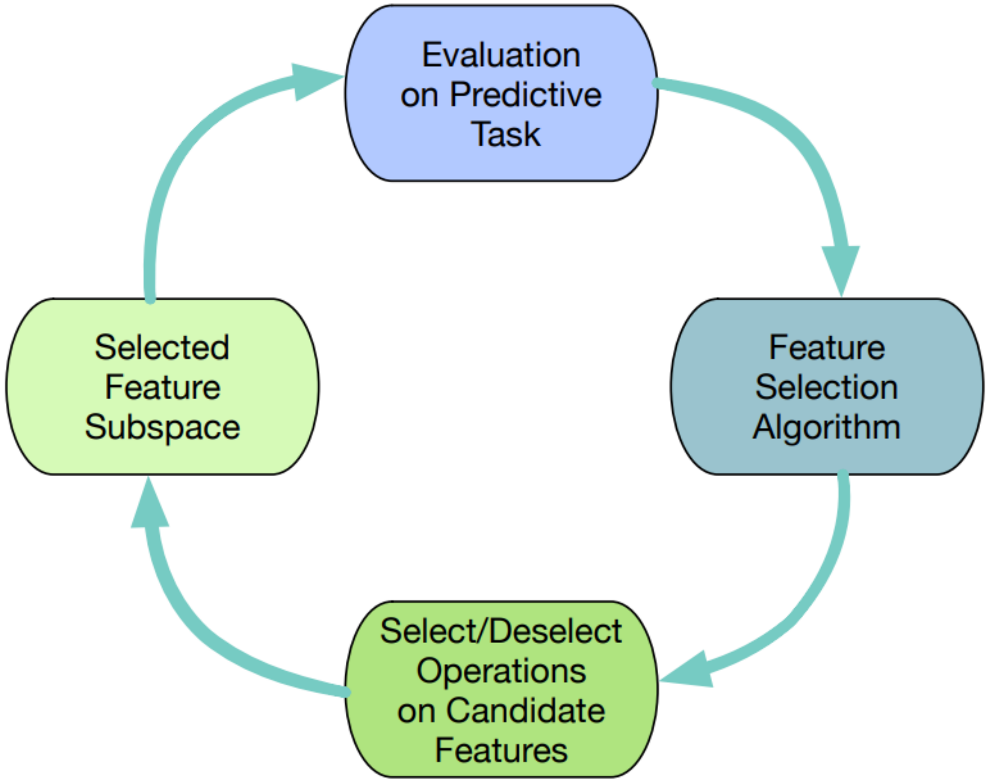
- Reducing the feature space by throwing out some of the features.
- Know which features are relevant, select an optimal subset of relevant features.

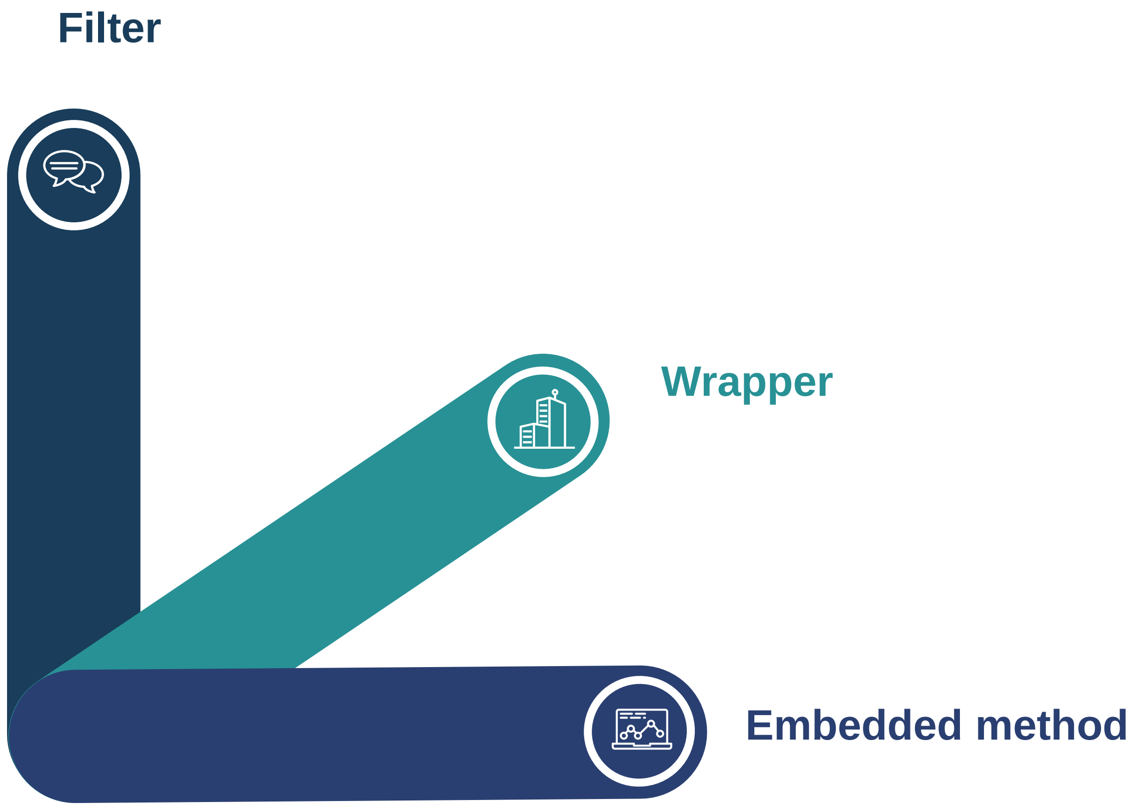
Why select features?

- Reduce dimensionality, improve prediction accuracy, increase comprehensibility, avoid overfitting.

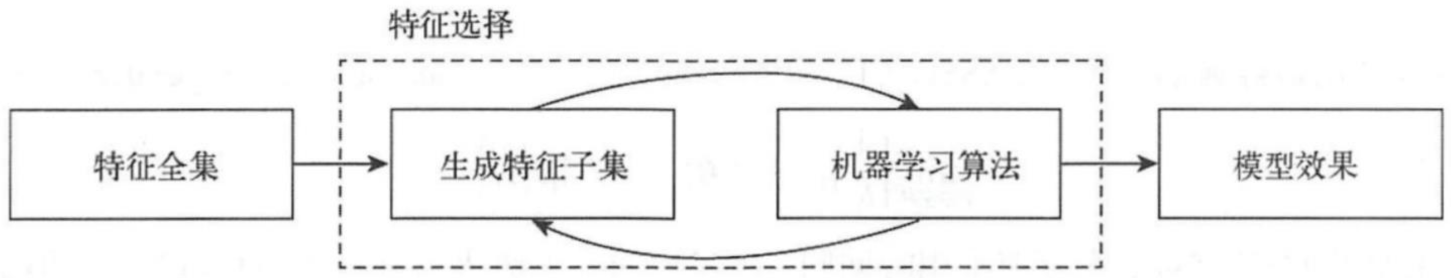
行星	周期（年）	平均距离	周期^2/距离^3
水星	0.241	0.39	0.98
金星	0.615	0.72	1.01
地球	1.00	1.00	1.00
火星	1.88	1.52	1.01
木星	11.8	5.20	0.99
土星	29.5	9.54	1.00
天王星	84.0	19.18	1.00
海王星	165	30.06	1.00

Feature Selection





Feature Selection

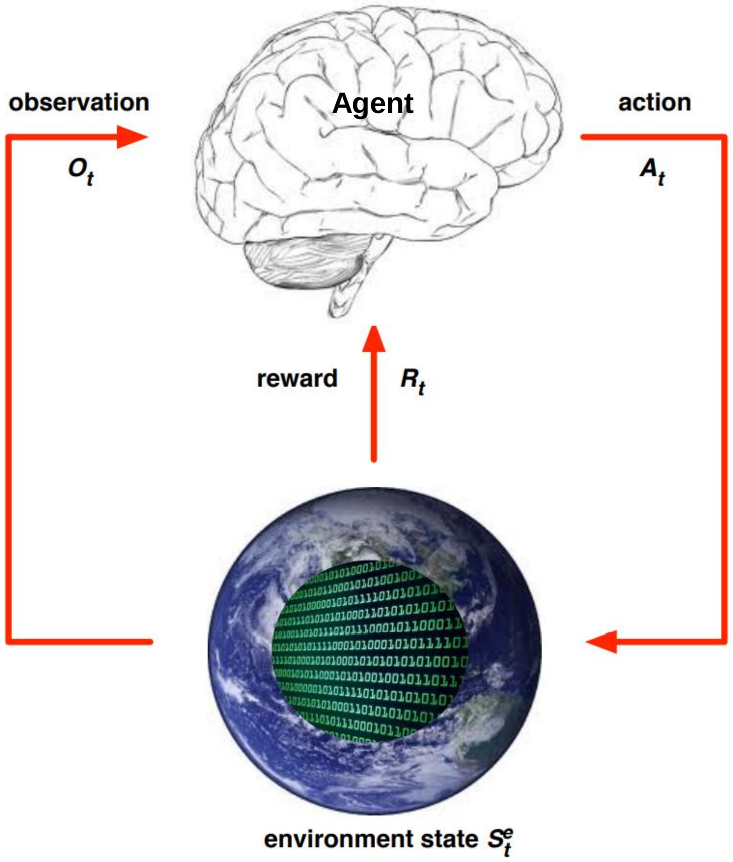


Algorithm name	Definition	Insufficient	Way
Filter method	Score the feature Select top K	Ignore the feature dependencies and interactions between feature selection and predictors	Variance、Pearson correlation coefficient
Wrapper method	By a search strategy that collaborates with predictive task	To search a very large feature space	Random search feature elimination
Embedded method	Integration of feature selection and learning training	Be subject to the strong structured assumptions of predictive task	Decision tree

Challenge

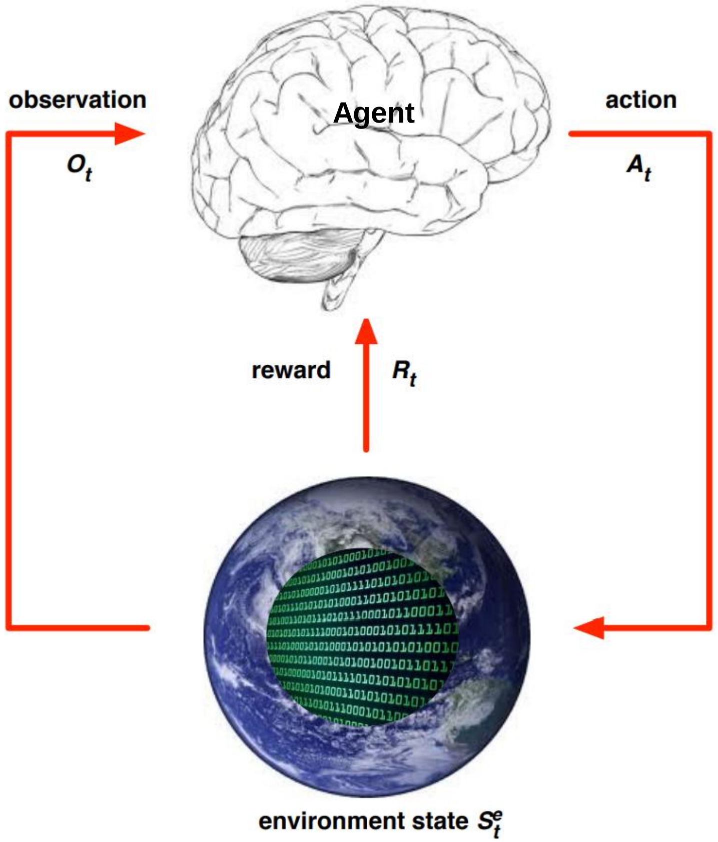
As can be seen, feature selection is a complicated process that requires:

- strategic design of feature significance measurement
- accelerated search of near-optimized feature subset (speed)
- meaningful integration of predictive models.



- At each step t the agent:
  - Executes action A_t
  - Receives observation O_t
  - Receives scalar reward R_t
- The environment:
  - Receives action A_t
  - Emits observation O_{t+1}
  - Emits scalar reward R_{t+1}
- t increments at env. step

Reinforcement Learning



Corresponding relationship

Multi-agent	→	Feature
Action	→	Select 1, deselect 0
Environment	Random select →	Feature subspace
State	→	Describe the selected feature subset
Reward	→	Acc, Rv, Rd

Framework

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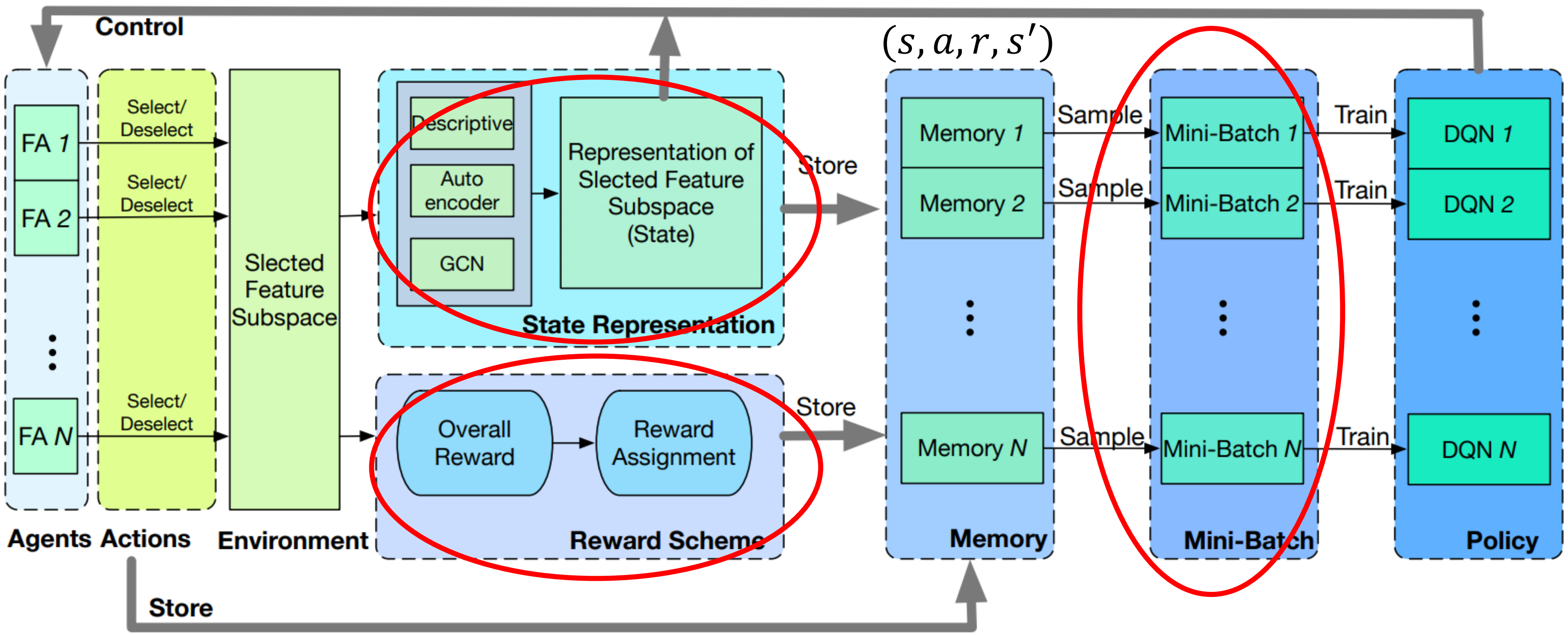
Framework

Control Stage

Training Stage



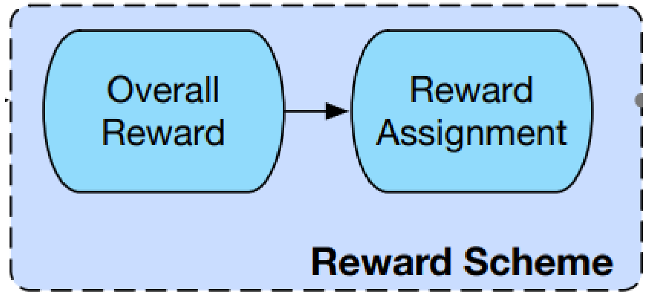
input

Current state

output

Action and next state

Reward



01. Predictive Accuracy

(TP+TN) / (TP+TN+FP+FN)

- TP：True Positive，样本为正例，且被判定为正，即真正
- FN：False Negative，样本为正例，但错误地被判定为负，即假负
- FP：False Positive，样本为负例，但错误地被判定为正，即假正
- TP：True Negative，样本为负例，且被判定为负，即真负

	分类为正例	分类为负例
实际为正例	TP	FN
实际为负例	FP	TN

02. Information redundancy

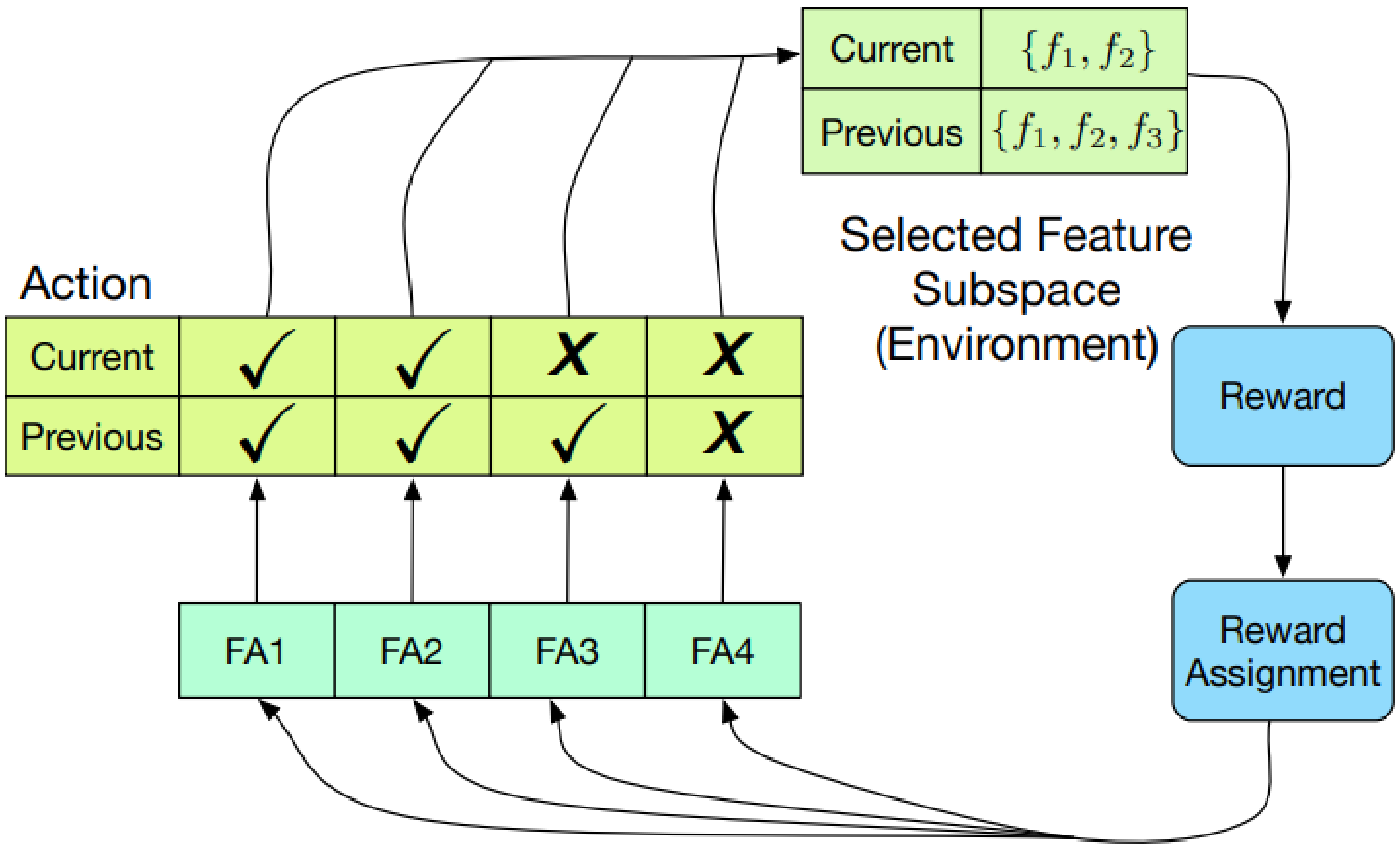
$$Rd = \frac{1}{|S|^2} \sum_{\boldsymbol{x_i}, \boldsymbol{x_j} \in S} \boldsymbol{I}(\boldsymbol{x_i}; \boldsymbol{x_j})$$

03. Information relevance

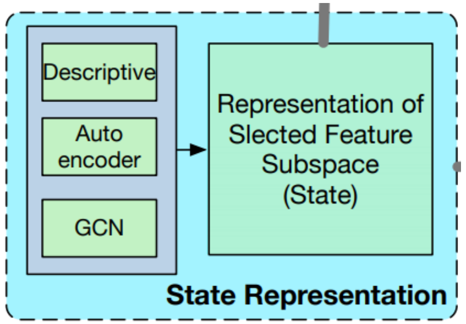
$$Rv = \frac{1}{|S|} \sum_{\boldsymbol{x_i} \in S} I(\boldsymbol{x_i}; \boldsymbol{c})$$

Reward

- Statistics of all the features in the last two rounds, without statistical times for average distribution.

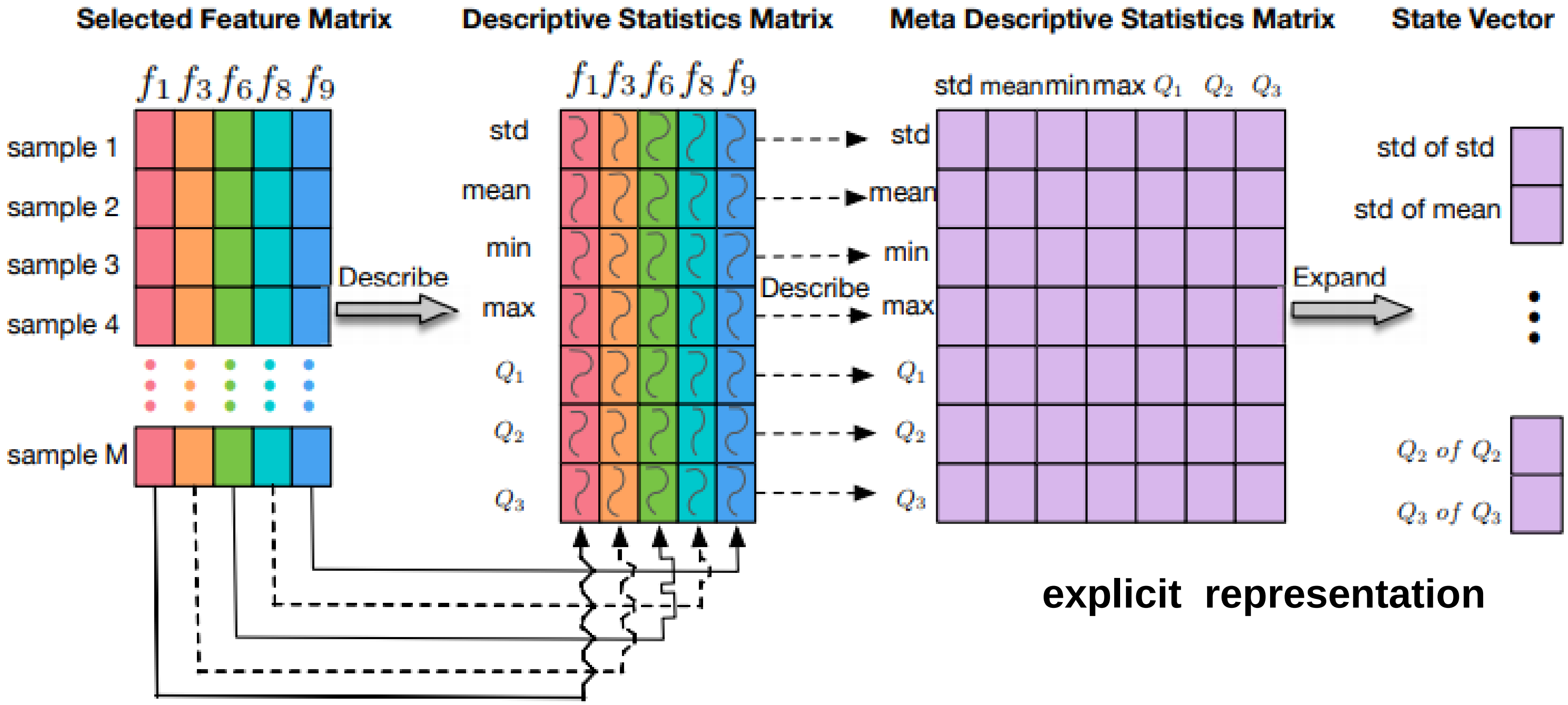


State Representation



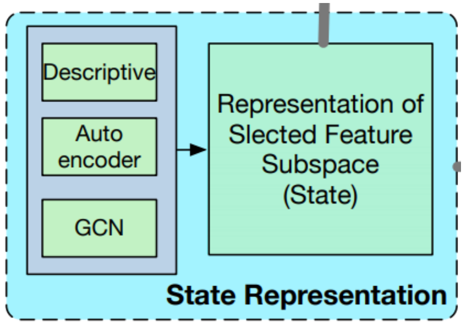
1.Meta descriptive statistics

- Step1 : from the column, extract seven descriptive statistics.
- Step2 : from the row, extract seven descriptive statistics.



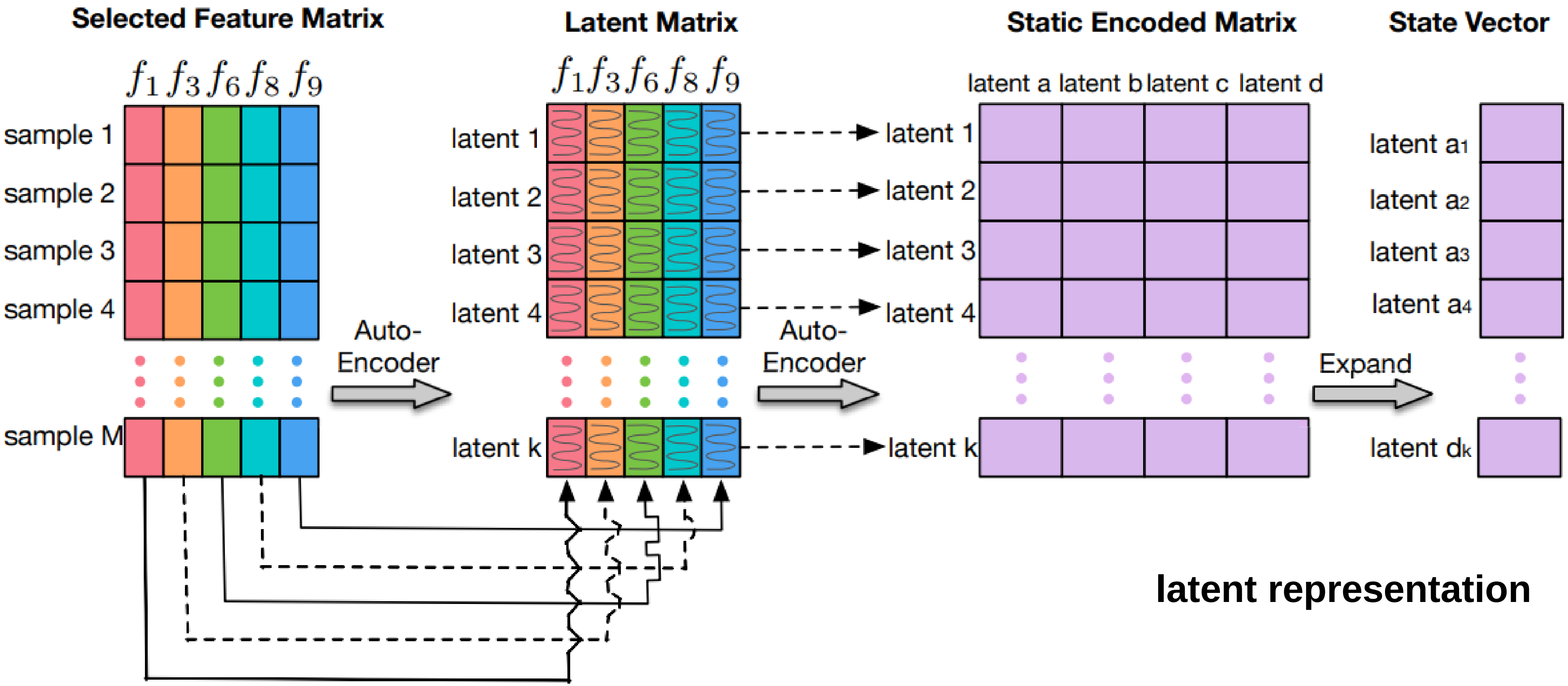
explicit representation

State Representation



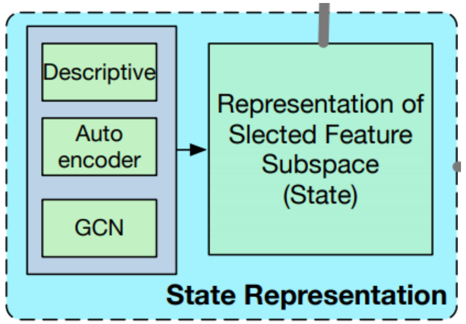
2. Autoencoder Based Deep Representation of Feature Subspace

- An autoencoder's encoder that maps the input into a latent representation, it has the fixed length.



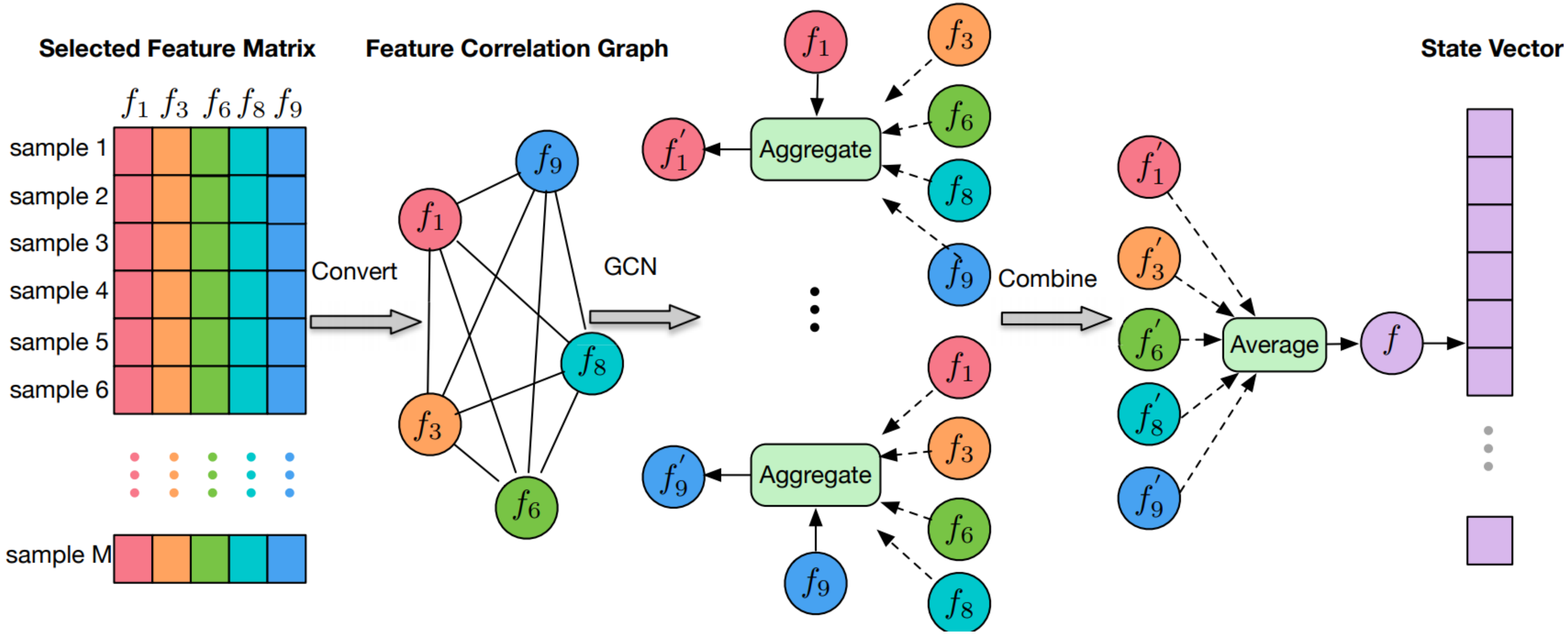
latent representation

State Representation



3 . Dynamic-Graph Based GCN

- Convert the selected Feature Matrix into a complete graph.
- GCN extracts the structure characteristics of the graph.
- Depend on the weight to Aggregate and average.



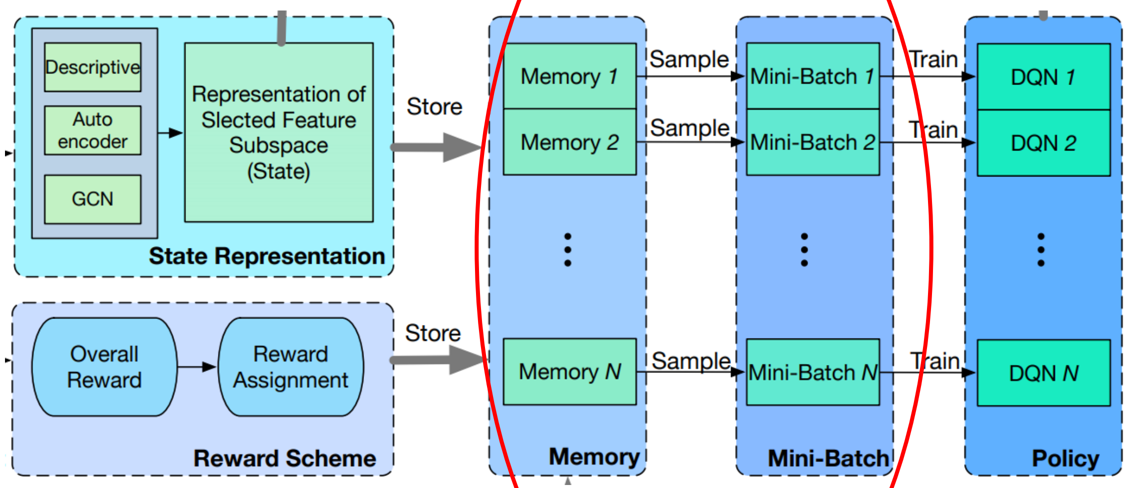
Correlations among features

GMM-Based Sample (Gaussian Mixture Model)

Algorithm 1: The GMM-Based Generative Rectified Sampling Algorithm

Input : Memory dataset T.
Output : A mini-batch of samples B.

$p \leftarrow$ high-quality sample proportion of T.
Stratify T into two groups. Samples with $a = 0$ are assigned to group T_0 and samples with $a = 1$ are assigned to group T_1.
for $i = 0$ *to* 1 **do**
  $N_i \leftarrow$ sample number of T_i.
  $K_i \leftarrow$ component number of GMM model $\mathcal{G}^i$.
  Rank samples in T_i by their reward r, then select top $N_i * p$ samples from T_i to form the high-quality dataset H_i.
  Use H_i to train the GMM $\mathcal{G}^i = \sum_1^{K_i} \phi_i \mathcal{N}(\mu_i, \Sigma_i)$ via EM algorithm.
  Generate $N_i * (1 - p)$ samples from G^i to form the generated dataset G_i.
  Join H_i and G_i to create high-quality dataset of action i, T_i'.
end
Join T_0' and T_1' to get high-quality dataset T'.
Sample a mini-batch of samples B from T'.



When the model contains hidden variables, maximum likelihood estimation is used to estimate the model parameters

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Evaluation

Basic content

Data : 15120 samples with 54 features(10 continuous, and 44 are categorical) from Kaggle.

Evaluation

Q1 **Accuracy**

Q2 **Precision**

- 指分类为正例的样本中，标签也为正例的样本比例
- 计算公式为TP/(TP+FP)

Q3 **Recall**

指标签为正例的样本中，被分类为正例的样本比例

计算公式为TP/(TP+FN)

Q4 **F-measure**

$$F=\frac{1}{\alpha\frac{1}{P}+(1-\alpha)\frac{1}{R}}=\frac{(\beta^2+1)PR}{\beta^2P+R}$$

- Performance
- Robustness Check
- Reward Function
- State Representation
- GMM based Generative Rectified Sampling

Robustness Check

		Predictors				
		RF	LASSO	DT	SVM	XGBoost
Algorithms	K-Best	0.7943	0.8246	0.8125	0.8324	0.8076
	mRMR	0.8042	0.8124	0.8096	0.8175	0.8239
	LASSO	0.8426	**0.8513**	0.8241	0.8131	0.8434
	RFE	0.8213	0.8236	0.8453	0.8257	0.8348
	GFS	0.8423	0.8318	0.8350	0.8346	0.8302
	SARLFS	0.8321	0.8295	0.8401	0.8427	0.8450
	MARLFS	**0.8690**	0.8424	**0.8583**	**0.8542**	**0.8731**

Overall accuracy of feature selection algorithms on different predictors

Reward Function

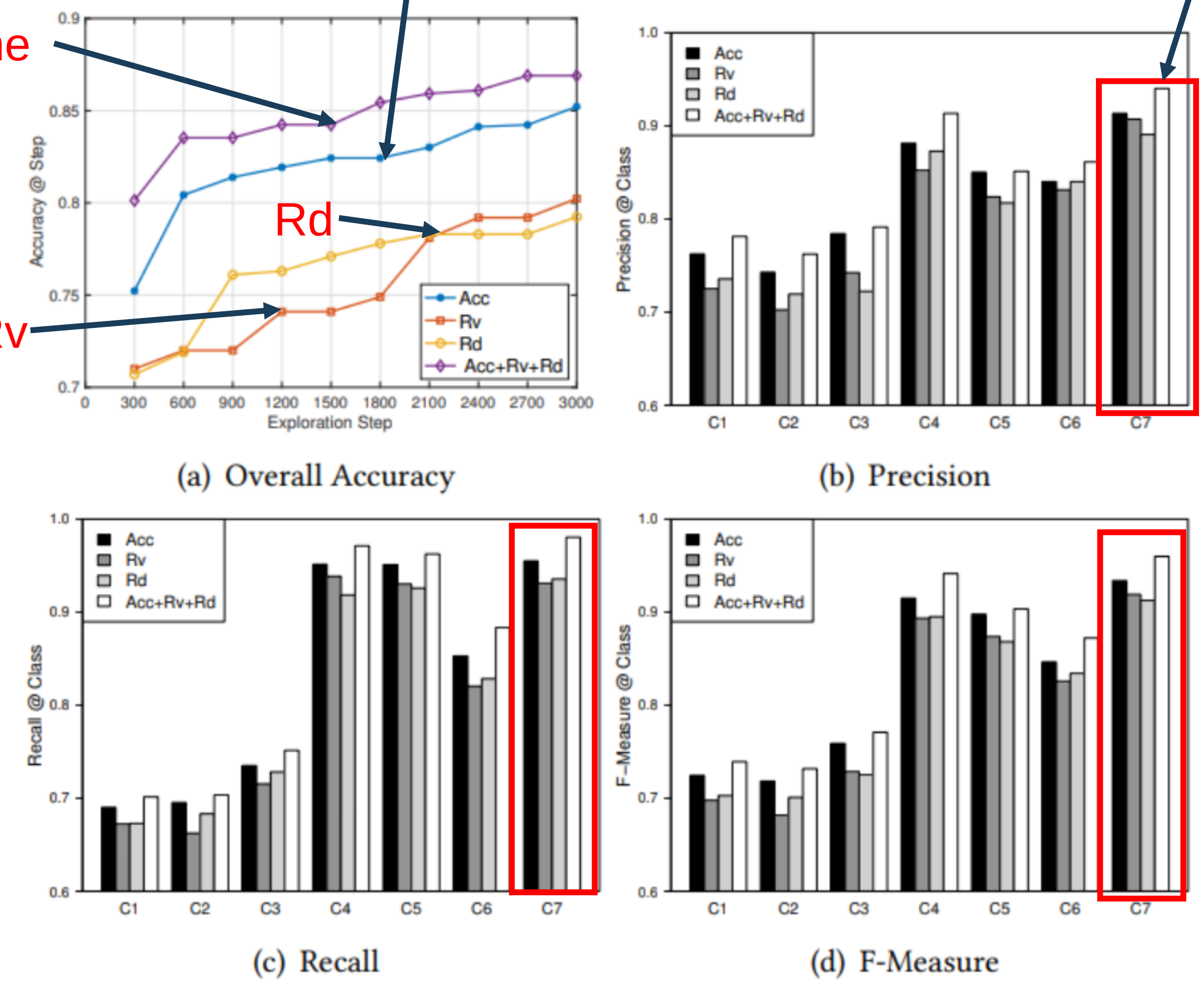
Acc

Acc、Rv、Rd、Combine

Combine

Rd

Rv



The highest performance

Seven Predictors(C1—C7)
Four Parameters

Performance comparison of different reward functions

Representation

Meta descriptive+Autoencoder

Combine

GCN

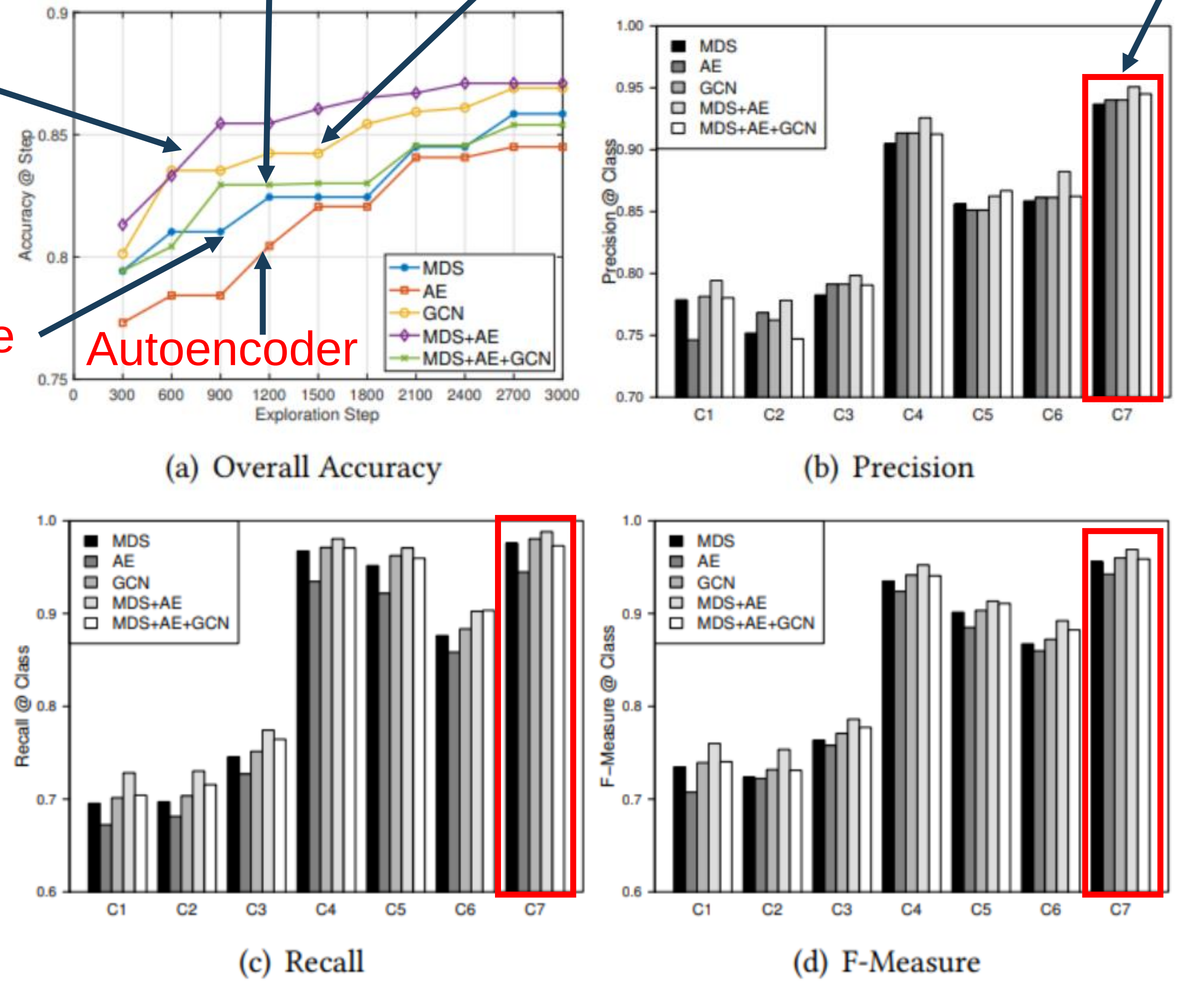
Meta descriptive

Autoencoder

MDS、AE、GCN、MDS+AS、Combine

The highest performance

This might be explained by the fact that there is potential training loss in the training phrase of AE and GCN

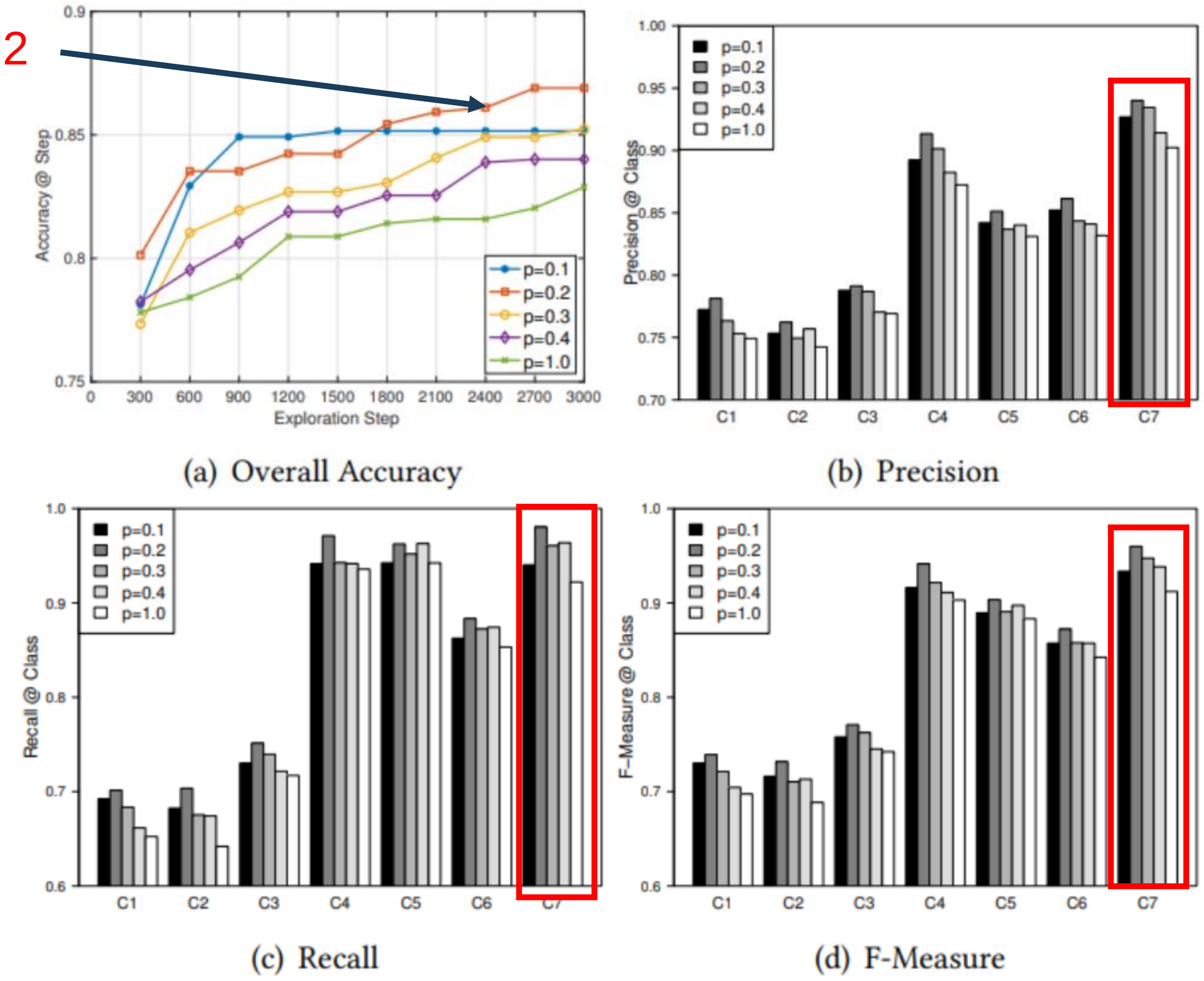


Performance comparison of different representation learning methods

Sample

Different the value of p

P = 0.2



P = 0.2 max

Performance comparison of different GMM sampling strategies

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Conclusion

Conclusion

Reformulate feature subspace exploration with a multi-agent RL framework and integrate the interactions between features into a new reward scheme.

We conduct extensive experiments to demonstrate the enhanced performances of our method

We develop three different methods to derive accurate state representation

We develop a GMM-based generative rectified sampling method to improve the training and exploration.

Thanks for your listening!