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Evaluation Metrics for Classification, Clustering, and Reinforcement Learning

1. Classification Evaluation Metrics

Evaluation metrics in classification quantify how well a predictive model assigns classes to instances. These metrics assess different dimensions such as correctness, error rate, class balance handling, and ranking ability.

1.1 Accuracy

Definition

Accuracy measures the proportion of correctly predicted instances out of all instances.

Formula

$$\text{Accuracy} = \frac{TP + TN}{TP + TN + FP + FN}$$

Interpretation

- Best used when classes are **balanced**.
- Misleading when dataset is **imbalanced**.

Python Implementation

```
from sklearn.metrics import accuracy_score  
accuracy = accuracy_score(y_true, y_pred)
```

1.2 Precision

Definition

Precision measures the proportion of predicted positives that are actually positive.

Formula

$$\text{Precision} = \frac{TP}{TP + FP}$$

Interpretation

- Useful when **false positives are costly** (e.g., spam detection).

Python

```
from sklearn.metrics import precision_score  
precision = precision_score(y_true, y_pred)
```

1.3 Recall (Sensitivity / True Positive Rate)

Definition

Recall indicates how many actual positive instances the classifier correctly identified.

Formula

$$\text{Recall} = \frac{TP}{TP + FN}$$

Interpretation

- Important when missing a positive instance is costly (e.g., disease detection).

Python

```
from sklearn.metrics import recall_score  
recall = recall_score(y_true, y_pred)
```

1.4 F1-Score

Definition

F1 score is the **harmonic mean** of Precision and Recall.

Formula

$$F1 = 2 \cdot \frac{\text{Precision} \cdot \text{Recall}}{\text{Precision} + \text{Recall}}$$

Interpretation

- Balances Precision and Recall.
- Useful for **imbalanced datasets**.

Python

```
from sklearn.metrics import f1_score
```

```
f1 = f1_score(y_true, y_pred)
```

1.5 Matthews Correlation Coefficient (MCC)

Definition

MCC measures the correlation between predicted and actual classes. It is considered one of the most reliable metrics for imbalanced classification.

Formula

$$MCC = \frac{TP \cdot TN - FP \cdot FN}{\sqrt{(TP + FP)(TP + FN)(TN + FP)(TN + FN)}}$$

Interpretation

- +1 → Perfect prediction
- 0 → Random prediction
- -1 → Completely wrong prediction

Python

```
from sklearn.metrics import matthews_corrcoef  
mcc = matthews_corrcoef(y_true, y_pred)
```

1.6 Precision–Recall Curve (PRC)

Definition

A curve showing the tradeoff between Precision and Recall across thresholds.

Key Points

- Useful for **highly imbalanced** datasets.
- Area under PR curve helps evaluate ranking ability.

Python

```
from sklearn.metrics import precision_recall_curve  
prec, rec, thr = precision_recall_curve(y_true, y_score)
```

1.7 ROC Curve & AUC

Definition

ROC curve plots True Positive Rate (TPR) vs. False Positive Rate (FPR).

Formula

$$TPR = \frac{TP}{TP + FN}$$
$$FPR = \frac{FP}{FP + TN}$$

AUC (Area Under Curve)

Evaluates the performance across all classification thresholds.

Interpretation

- AUC = 1 → Perfect classifier
- AUC = 0.5 → Random
- AUC < 0.5 → Worse than random

Python

```
from sklearn.metrics import roc_auc_score  
auc = roc_auc_score(y_true, y_score)
```

2. Clustering Evaluation Metrics

Clustering metrics are divided into:

- **Internal Metrics** → Do not require ground truth labels
- **External Metrics** → Require true labels for comparison

2.1 Internal Clustering Metrics

These evaluate the quality of clusters based on the structure of the dataset itself.

2.1.1 Silhouette Score

Definition

Measures how well each point fits within its cluster.

Formula

$$S = \frac{b - a}{\max(a, b)}$$

Where:

- **a** = average intra-cluster distance
- **b** = nearest-cluster distance

Interpretation

- +1 → Well-clustered
- 0 → Overlapping
- Negative → Wrong cluster

Python

```
from sklearn.metrics import silhouette_score  
sil = silhouette_score(X, labels)
```

2.1.2 Davies–Bouldin Index (DBI)

Definition

Measures average similarity between clusters (lower is better).

Formula

$$DBI = \frac{1}{k} \sum_{i=1}^k \max_{j \neq i} \left(\frac{\sigma_i + \sigma_j}{d(c_i, c_j)} \right)$$

Python

```
from sklearn.metrics import davies_bouldin_score  
dbi = davies_bouldin_score(X, labels)
```

2.1.3 Dunn Index

Definition

Measures separation and compactness.

Formula

$$D = \frac{\text{Minimum inter-cluster distance}}{\text{Maximum intra-cluster distance}}$$

Interpretation

Higher Dunn index → Better clustering

(No built-in sklearn function)

2.2 External Clustering Metrics

These compare cluster labels with true labels.

2.2.1 Rand Index

Definition

Measures similarity between predicted and true labels.

Formula

$$RI = \frac{TP + TN}{TP + TN + FP + FN}$$

2.2.2 Adjusted Rand Index (ARI)

Definition

Corrects Rand Index for chance.

Python

```
from sklearn.metrics import adjusted_rand_score  
ari = adjusted_rand_score(y_true, labels)
```

2.2.3 Homogeneity Score

Definition

Measures whether each cluster contains only members of a single class.

Python

```
from sklearn.metrics import homogeneity_score  
homo = homogeneity_score(y_true, labels)
```

2.2.4 Completeness Score

Definition

Measures whether all members of a class are assigned to the same cluster.

Python

```
from sklearn.metrics import completeness_score  
comp = completeness_score(y_true, labels)
```

2.2.5 V-Measure

Definition

Harmonic mean of Homogeneity and Completeness.

Python

```
from sklearn.metrics import v_measure_score  
v = v_measure_score(y_true, labels)
```

2.2.6 RMSE (Root Mean Square Error)

Definition

Measures reconstruction error in centroid-based clustering (e.g., K-Means).

Formula

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (x_i - c_{label(i)})^2}$$

3. Reinforcement Learning Evaluation Metrics

Reinforcement Learning metrics evaluate policy quality, reward efficiency, and learning stability.

3.1 Cumulative Reward / Return

Definition

Total reward accumulated by the agent.

Discounted Return Formula

$$G_t = \sum_{k=0}^{\infty} \gamma^k R_{t+k+1}$$

3.2 Value Function Error

Definition

Measures how far estimated value function is from true value.

Formula

$$MSE = \frac{1}{n} \sum (V(s) - V^\pi(s))^2$$

3.3 Policy Loss

Definition

Measures how well the policy improves over iterations.

General Formula (Policy Gradient)

$$L(\theta) = -\mathbb{E}_{\pi_\theta} [\log \pi_\theta(a | s) A(s, a)]$$

Lower loss → Better policy

3.4 Additional Important RL Metrics

Success Rate

Percentage of times agent achieves the goal.

Episode Length

Number of steps per episode.

Stability (Variance of Reward)

Measures consistency.

GITHUB:

<https://github.com/sultanali543/Evaluation-Metrics-for-Classification-Clustering-and-Reinforcement-Learning>

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