

Cheat Sheet: Evaluating and Validating Machine Learning Models

Model evaluation metrics and methods

Method Name	Description	Code Syntax
classification_report	<p>Generates a report with precision, recall, F1-score, and support for each class in classification problems. Useful for model evaluation.</p> <p>Hyperparameters: target_names: List of labels to include in the report.</p> <p>Pros: Provides a comprehensive evaluation of classification models.</p> <p>Limitations: May not provide enough insight for imbalanced datasets.</p>	<pre>from sklearn.metrics import classification_report # y_true: True labels # y_pred: Predicted labels # target_names: List of target class names report = classification_report(y_true, y_pred, target_names=["class1", "class2"])</pre>
confusion_matrix	<p>Computes a confusion matrix to evaluate the classification performance, showing counts of true positives, false positives, true negatives, and false negatives.</p> <p>Hyperparameters: labels: List of class labels to include.</p> <p>Pros: Essential for understanding classification errors.</p> <p>Limitations: Doesn't give insights into prediction probabilities.</p>	<pre>from sklearn.metrics import confusion_matrix # y_true: True labels # y_pred: Predicted labels conf_matrix = confusion_matrix(y_true, y_pred)</pre>
mean_squared_error	<p>Calculates the mean squared error (MSE), a common metric for regression models. Lower values indicate better performance.</p> <p>Hyperparameters: sample_weight: Weights to apply to each sample.</p> <p>Pros: Simple and widely used metric.</p> <p>Limitations: Sensitive to outliers, as large errors are squared.</p>	<pre>from sklearn.metrics import mean_squared_error # y_true: True values # y_pred: Predicted values # sample_weight: Optional, array of sample weights mse = mean_squared_error(y_true, y_pred)</pre>
root_mean_squared_error	<p>Calculates the root mean squared error (RMSE), which is the square root of the MSE. RMSE gives more interpretable results as it is in the same units as the target.</p> <p>Hyperparameters: sample_weight: Weights to apply to each sample.</p> <p>Pros: More interpretable than MSE.</p> <p>Limitations: Like MSE, it can be sensitive to large errors and outliers.</p>	<pre>from sklearn.metrics import root_mean_squared_error # y_true: True values # y_pred: Predicted values # sample_weight: Optional, array of sample weights rmse = root_mean_squared_error(y_true, y_pred)</pre>

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mean_absolute_error	<p>Measures the average magnitude of errors in predictions, without considering their direction. Useful for understanding the average error size.</p> <p>Hyperparameters: sample_weight: Optional sample weights.</p> <p>Pros: Less sensitive to outliers compared to MSE.</p> <p>Limitations: Does not penalize large errors as much as MSE or RMSE.</p>	<pre>from sklearn.metrics import mean_absolute_error # y_true: True values # y_pred: Predicted values mae = mean_absolute_error(y_true, y_pred)</pre>
r2_score	<p>Computes the coefficient of determination (R^2), which represents the proportion of variance explained by the model. A higher value indicates a better fit.</p> <p>Pros: Provides a clear indication of model performance.</p> <p>Limitations: Doesn't always represent model quality, especially for non-linear models.</p>	<pre>from sklearn.metrics import r2_score # y_true: True values # y_pred: Predicted values r2 = r2_score(y_true, y_pred)</pre>
silhouette_score	<p>Measures the quality of clustering by assessing the cohesion within clusters and separation between clusters. Higher scores indicate better clustering.</p> <p>Hyperparameters: metric: Distance metric to use.</p> <p>Pros: Useful for validating clustering performance.</p> <p>Limitations: Sensitive to outliers and choice of distance metric.</p>	<pre>from sklearn.metrics import silhouette_score # X: Data used in clustering # labels: Cluster labels for each sample score = silhouette_score(X, labels, metric='euclidean')</pre>
silhouette_samples	<p>Provides silhouette scores for each individual sample, indicating how well it fits its assigned cluster.</p> <p>Hyperparameters: metric: Distance metric to use.</p> <p>Pros: Offers granular insight into each sample's clustering quality.</p> <p>Limitations: Same as silhouette_score; sensitive to outliers and distance metric.</p>	<pre>from sklearn.metrics import silhouette_samples # X: Data used in clustering # labels: Cluster labels for each sample samples = silhouette_samples(X, labels, metric='euclidean')</pre>
davies_bouldin_score	<p>Measures the average similarity ratio of each cluster with the most similar cluster. Lower values indicate better clustering.</p> <p>Pros: Provides a simple, effective clustering evaluation.</p> <p>Limitations: May not work well with highly imbalanced clusters.</p>	<pre>from sklearn.metrics import davies_bouldin_score # X: Data used in clustering # labels: Cluster labels for each sample db_score = davies_bouldin_score(X, labels)</pre>

Voronoi	Computes the Voronoi diagram, which partitions space based on the nearest neighbor. Pros: Useful for spatial analysis and clustering. Limitations: Limited to use cases that involve spatial partitioning of data.	<pre>from scipy.spatial import Voronoi # points: Coordinates for Voronoi diagram vor = Voronoi(points)</pre>
voronoi_plot_2d	Plots the Voronoi diagram in 2D for visualizing clustering results. Hyperparameters: show_vertices: Whether to display the vertices. Pros: Great for visualizing spatial clustering. Limitations: Limited to 2D spaces and large datasets may cause performance issues.	<pre>from scipy.spatial import voronoi_plot_2d # vor: Voronoi diagram object voronoi_plot_2d(vor, show_vertices=True)</pre>
matplotlib.patches.Patch	Creates custom shapes such as rectangles, circles, or ellipses for adding to plots. Hyperparameters: color: Fills color of the shape. Pros: Versatile for visual customization. Limitations: May not support all shapes or complex customizations.	<pre>import matplotlib.patches as patches # Create a rectangle with specified width, height, and position rectangle = patches.Rectangle((0, 0), 1, 1, color='blue')</pre>
explained_variance_score	Measures the proportion of variance explained by the model's predictions. A higher score indicates better performance. Pros: Helps in assessing the fit of regression models. Limitations: Not suitable for classification tasks.	<pre>from sklearn.metrics import explained_variance_score # y_true: True values # y_pred: Predicted values ev_score = explained_variance_score(y_true, y_pred)</pre>
Ridge regression	Performs ridge regression (L2 regularization) to avoid overfitting by penalizing large coefficients. Hyperparameters: alpha: Regularization strength.	<pre>from sklearn.linear_model import Ridge # alpha: Regularization strength (larger values indicate stronger regularization) ridge = Ridge(alpha=1.0)</pre>

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	<p>Pros: Helps reduce overfitting in regression models.</p> <p>Limitations: May not work well with sparse data.</p>	
Lasso regression	<p>Performs lasso regression (L1 regularization), which encourages sparsity by penalizing the absolute value of coefficients.</p> <p>Hyperparameters: alpha: Regularization strength.</p> <p>Pros: Encourages sparse solutions, useful for feature selection.</p> <p>Limitations: May struggle with multicollinearity.</p>	<pre>from sklearn.linear_model import Lasso # alpha: Regularization strength (larger values indicate stronger regularization) lasso = Lasso(alpha=0.1)</pre>
Pipeline	<p>Chains multiple steps of preprocessing and modeling into a single object, ensuring efficient workflow.</p> <p>Pros: Simplifies code, ensures reproducibility.</p> <p>Limitations: May not work well with complex pipelines requiring dynamic configurations.</p>	<pre>from sklearn.pipeline import Pipeline # steps: List of tuples with name and estimator/transformer pipeline = Pipeline(steps=[('scaler', StandardScaler()), ('model', Ridge(alpha=1.0))])</pre>
GridSearchCV	<p>Performs exhaustive search over a specified parameter grid to find the best model configuration.</p> <p>Hyperparameters: param_grid: Dictionary of parameter grids.</p> <p>Pros: Ensures optimal model parameters.</p> <p>Limitations: Computationally expensive for large grids.</p>	<pre>from sklearn.model_selection import GridSearchCV # estimator: Model to be tuned # param_grid: Dictionary with parameters to search over grid_search = GridSearchCV(estimator=Ridge(), param_grid={'alpha': [0.1, 1.0, 10.0]})</pre>

Visualization strategies for k-means evaluation

Process Name	Brief Description	Code Snippet
Multiple runs of k-means	<p>Executes KMeans clustering multiple times with different random initializations to assess variability in cluster assignments.</p> <p>Advantage: Helps visualize consistency.</p> <p>Limitation: Computationally costly for large datasets.</p>	<pre># Number of runs for KMeans with different random states n_runs = 4 inertia_values = [] plt.figure(figsize=(12, 12)) # Run K-Means multiple times with different random states for i in range(n_runs): kmeans = KMeans(n_clusters=4, random_state=None) # Use the default `n_init` kmeans.fit(X) inertia_values.append(kmeans.inertia_) # Plot the clustering result plt.subplot(2, 2, i + 1) plt.scatter(X[:, 0], X[:, 1], c=kmeans.labels_, cmap='tab10', alpha=0.6, edgecolor='k') plt.scatter(kmeans.cluster_centers[:, 0], kmeans.cluster_centers[:, 1], c='red', s=200, marker='x', label='Centroids') plt.title(f'K-Means Clustering Run {i + 1}')</pre>

		<pre> plt.xlabel('Feature 1') plt.ylabel('Feature 2') plt.legend() plt.tight_layout() plt.show() # Print inertia values for i, inertia in enumerate(inertia_values, start=1): print(f'Run {i}: Inertia={inertia:.2f}') </pre>
Elbow method	<p>Evaluates the optimal number of clusters by plotting inertia (within-cluster sum of squares) for different k values.</p> <p>Advantage: Easy to interpret.</p> <p>Limitation: Subjective elbow point.</p>	<pre> # Range of k values to test k_values = range(2, 11) # Store performance metrics inertia_values = [] for k in k_values: kmeans = KMeans(n_clusters=k, random_state=42) y_kmeans = kmeans.fit_predict(X) # Calculate and store metrics inertia_values.append(kmeans.inertia_) # Plot the inertia values (Elbow Method) plt.figure(figsize=(18, 6)) plt.subplot(1, 3, 1) plt.plot(k_values, inertia_values, marker='o') plt.title('Elbow Method: Inertia vs. k') plt.xlabel('Number of Clusters (k)') plt.ylabel('Inertia') </pre>
Silhouette method	<p>Determines the optimal number of clusters by evaluating Silhouette Scores for different k values.</p> <p>Advantage: Considers both cohesion and separation.</p> <p>Limitation: High computation for large datasets.</p>	<pre> # Range of k values to test k_values = range(2, 11) # Store performance metrics silhouette_scores = [] for k in k_values: kmeans = KMeans(n_clusters=k, random_state=42) y_kmeans = kmeans.fit_predict(X) silhouette_scores.append(silhouette_score(X, y_kmeans)) # Plot the Silhouette Scores plt.figure(figsize=(18, 6)) plt.subplot(1, 3, 2) plt.plot(k_values, silhouette_scores, marker='o') plt.title('Silhouette Score vs. k') plt.xlabel('Number of Clusters (k)') plt.ylabel('Silhouette Score') </pre>

Davies-Bouldin Index	<p>Evaluates clustering performance by calculating DBI for different k values.</p> <p>Advantage: Quantifies compactness and separation.</p> <p>Limitation: Sensitive to cluster shapes and density.</p>	<pre># Range of k values to test k_values = range(2, 11) # Store performance metrics davies_bouldin_indices = [] for k in k_values: kmeans = KMeans(n_clusters=k, random_state=42) y_kmeans = kmeans.fit_predict(X) davies_bouldin_indices.append(davies_bouldin_score(X, y_kmeans)) # Plot the Davies-Bouldin Index plt.figure(figsize=(18, 6)) plt.subplot(1, 3, 3) plt.plot(k_values, davies_bouldin_indices, marker='o') plt.title('Davies-Bouldin Index vs. k') plt.xlabel('Number of Clusters (k)') plt.ylabel('Davies-Bouldin Index')</pre>
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