

# 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><b>Hyperparameters:</b> target_names: List of labels to include in the report.</p> <p><b>Pros:</b> Provides a comprehensive evaluation of classification models.</p> <p><b>Limitations:</b> 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><b>Hyperparameters:</b> labels: List of class labels to include.</p> <p><b>Pros:</b> Essential for understanding classification errors.</p> <p><b>Limitations:</b> 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><b>Hyperparameters:</b> sample_weight: Weights to apply to each sample.</p> <p><b>Pros:</b> Simple and widely used metric.</p> <p><b>Limitations:</b> 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><b>Hyperparameters:</b> sample_weight: Weights to apply to each sample.</p> <p><b>Pros:</b> More</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>

	<p>interpretable than MSE.</p> <p><b>Limitations:</b> Like MSE, it can be sensitive to large errors and outliers.</p>	
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><b>Hyperparameters:</b> sample_weight: Optional sample weights.</p> <p><b>Pros:</b> Less sensitive to outliers compared to MSE.</p> <p><b>Limitations:</b> 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 (<math>R^2</math>), which represents the proportion of variance explained by the model. A higher value indicates a better fit.</p> <p><b>Pros:</b> Provides a clear indication of model performance.</p> <p><b>Limitations:</b> 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><b>Hyperparameters:</b> metric: Distance metric to use.</p> <p><b>Pros:</b> Useful for validating clustering performance.</p> <p><b>Limitations:</b> 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><b>Hyperparameters:</b> metric: Distance metric to use.</p> <p><b>Pros:</b> Offers granular insight into each sample's clustering quality.</p> <p><b>Limitations:</b> 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</p>	<pre>from sklearn.metrics import davies_bouldin_score # X: Data used in clustering # labels: Cluster labels for each sample</pre>

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

	overfitting in regression models. <b>Limitations:</b> May not work well with sparse data.	
Lasso regression	Performs lasso regression (L1 regularization), which encourages sparsity by penalizing the absolute value of coefficients. <b>Hyperparameters:</b> alpha: Regularization strength. <b>Pros:</b> Encourages sparse solutions, useful for feature selection. <b>Limitations:</b> May struggle with multicollinearity.	<pre>from sklearn.linear_model import Lasso # alpha: Regularization strength (larger values indicate stronger regularization) lasso = Lasso(alpha=0.1)</pre>
Pipeline	Chains multiple steps of preprocessing and modeling into a single object, ensuring efficient workflow. <b>Pros:</b> Simplifies code, ensures reproducibility. <b>Limitations:</b> May not work well with complex pipelines requiring dynamic configurations.	<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	Performs exhaustive search over a specified parameter grid to find the best model configuration. <b>Hyperparameters:</b> param_grid: Dictionary of parameter grids. <b>Pros:</b> Ensures optimal model parameters. <b>Limitations:</b> Computationally expensive for large grids.	<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	Executes KMeans clustering multiple times with different random initializations to assess variability in cluster assignments.  <b>Advantage:</b> Helps visualize consistency.  <b>Limitation:</b> Computationally costly for large datasets.	<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_[i, 0], kmeans.cluster_centers_[i, 1], c='red', s=200, marker='x') plt.title(f'K-Means Clustering Run {i + 1}') 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>

<b>Elbow method</b>	<p>Evaluates the optimal number of clusters by plotting inertia (within-cluster sum of squares) for different <b>k</b> values.</p> <p><b>Advantage:</b> Easy to interpret.</p> <p><b>Limitation:</b> 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>
<b>Silhouette method</b>	<p>Determines the optimal number of clusters by evaluating Silhouette Scores for different <b>k</b> values.</p> <p><b>Advantage:</b> Considers both cohesion and separation.</p> <p><b>Limitation:</b> 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>
<b>Davies-Bouldin Index</b>	<p>Evaluates clustering performance by calculating DBI for different <b>k</b> values.</p> <p><b>Advantage:</b> Quantifies compactness and separation.</p> <p><b>Limitation:</b> 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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