




# Basics of Machine Learning

1. Supervised ML Concepts
2. Unsupervised ML concepts
3. Overfitting, Bias, Validation, Metrics
4. Basic Data Handling skill

## Supervised Machine Learning (ML) Concepts:

Supervised ML involves training a model on **labeled data** (input-output pairs).

### Key Concepts:

-  Input (features) + Output (labels)
-  Model learns from training data to predict labels on unseen data
-  Examples: Classification (Spam/Not Spam), Regression (Price Prediction)

### Definition:

Supervised learning is a type of machine learning where an algorithm learns from labeled data. "Labeled" data means that each data point is associated with a corresponding output or "target" value.

The goal is to learn a mapping function that can predict the output for new, unseen input data.

### Key Concepts:

- Labeled Data: The cornerstone of supervised learning.
- Training Data: The dataset used to train the model.
- Features: The input variables used to predict the output.
- Labels/Targets: The output variables that the model is trying to predict.

### Algorithms:

Common supervised learning algorithms include:

- Linear Regression (for predicting continuous values)
- Logistic Regression (for classification)
- Decision Trees
- Random Forests
- Support Vector Machines (SVMs)
- Neural Networks

### Applications:

- Image classification
- Predicting house prices
- Medical diagnosis

- Spam detection

## Unsupervised Machine Learning (ML):

### Definition:

Unsupervised learning is a type of machine learning where an algorithm learns from unlabeled data.

The goal is to discover hidden patterns or structures in the data.

### Key Concepts:

Unlabeled Data: The input data without corresponding output labels.

Clustering: Grouping similar data points.

Dimensionality Reduction: Reducing the number of variables in a dataset.

### Algorithms:

Common unsupervised learning algorithms include:

- K-means clustering
- Hierarchical clustering
- Principal Component Analysis 1 (PCA)
- Autoencoders

### Applications:

- Customer segmentation
- Anomaly detection
- Image compression
- Recommendation systems

## Validation

Validation in **Machine Learning (ML)** refers to evaluating a model's performance to ensure that it generalizes well to unseen data.

### 1. Train-Test Split

A simple method where the dataset is split into two subsets:

- **Training set:** Used to train the model.
- **Test set:** Used to evaluate the model's performance on unseen data.

## # Stratified K-Fold Validation

Stratified K-Fold validation is a cross-validation technique that preserves the class distribution in each fold, making it particularly useful for imbalanced datasets.

### ## How It Works

1. **\*\*Splitting Process\*\***: The dataset is divided into K folds (subsets) while maintaining the same percentage of samples for each class as in the original

dataset.

2. **Iteration**: The process runs K times, with each fold as the test set exactly once while the remaining K-1 folds form the training set.

3. **Evaluation**: The model is trained and evaluated K times, with the final performance typically being the average of all K evaluations.

## ## Key Advantages

- **Preserves Class Distribution**: Especially important for imbalanced datasets
- **Reduces Variance**: Provides more reliable performance estimates
- **Comprehensive Evaluation**: Every data point gets to be in the test set exactly once

## ## Implementation in Python

```
```python
from sklearn.model_selection import StratifiedKFold
from sklearn.datasets import load_iris
from sklearn.linear_model import LogisticRegression
from sklearn.metrics import accuracy_score

# Load dataset
X, y = load_iris(return_X_y=True)

# Initialize Stratified K-Fold
skf = StratifiedKFold(n_splits=5, shuffle=True, random_state=42)

# Initialize model
model = LogisticRegression()

# Perform cross-validation
accuracies = []
for train_index, test_index in skf.split(X, y):
    X_train, X_test = X[train_index], X[test_index]
    y_train, y_test = y[train_index], y[test_index]

    model.fit(X_train, y_train)
    y_pred = model.predict(X_test)
    accuracies.append(accuracy_score(y_test, y_pred))

print(f"Average accuracy: {sum(accuracies)/len(accuracies):.4f}")
```
```

## ## When to Use

- With classification problems (especially with imbalanced classes)
- When you need reliable performance estimates
- When dataset size is limited

## ## Comparison with Regular K-Fold

- Regular K-Fold doesn't maintain class proportions
- Stratified K-Fold is generally preferred for classification
- Regular K-Fold may be sufficient for regression problems or balanced datasets

## ### \*\*Intuitive Explanation of Stratified K-Fold Validation\*\*

Imagine you're a teacher dividing your class into **5 study groups** for a series of quizzes. Your class has:

- **60% "A" students** (high performers)
- **30% "B" students** (average performers)
- **10% "C" students** (struggling)

If you split them randomly into groups, some groups might accidentally get **too many "A" students**, while others get **too many "C" students**. This would make some quizzes unfairly easy or hard, and your evaluation of the groups' performance wouldn't be reliable.

### #### \*\*What Stratified K-Fold Does:\*\*

Instead of random splitting, **Stratified K-Fold ensures that each group has the same ratio of A, B, and C students as the whole class** (60% A, 30% B, 10% C).

#### **This way:**

- Every quiz (test fold) is **representative** of the whole class.
- No group gets an unfair advantage or disadvantage.
- The average performance across all quizzes gives a **true estimate** of how well the teacher's methods work.

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## ### \*\*Real-World Machine Learning Example\*\*

Suppose you have:

- A dataset of **1000 patients**, where:
  - **900 are healthy** (class 0)

- **100** have a disease (class 1)

If you use **normal K-Fold**, some folds might get **too few (or zero) disease cases**, making model evaluation unreliable.

### **But Stratified K-Fold ensures:**

- Each fold has **90% healthy & 10% disease cases**, just like the original data.
- The model is fairly tested on all types of data.

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### **Key Takeaway**

Stratified K-Fold is like a **fair referee** ensuring every test round has the right mix of classes, so your model's performance isn't skewed by luck.

**Use it when:**

- ✓ You have **imbalanced classes** (e.g., fraud detection, rare diseases).
- ✓ You want **reliable performance estimates** without randomness affecting results.

## **Practical Example of Stratified K-Fold Validation**

Let's walk through a real-world scenario step by step using Python and a sample dataset.

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### **Scenario: Predicting Loan Defaults (Imbalanced Data)**

We'll use a dataset where:

- **Most people repay loans** (class 0 = 90%)
- **A few default** (class 1 = 10%)

#### **Step 1: Load and Inspect the Data**

```
python
import numpy as np
from sklearn.datasets import make_classification

# Create an imbalanced dataset (90% non-default, 10% default)
X, y = make_classification(
    n_samples=1000,
    n_classes=2,
    weights=[0.9, 0.1], # 90% class 0, 10% class 1
    random_state=42
)

# Check class distribution
```

```
print("Class distribution:", np.bincount(y))
...
```

```
**Output:**
...
```

```
Class distribution: [900 100] # 900 non-defaults, 100 defaults
...
```

---

### #### \*\*Step 2: Apply Stratified K-Fold\*\*

We'll split the data into **5 folds** while preserving the 90:10 ratio in each fold.

```
```python
from sklearn.model_selection import StratifiedKFold

skf = StratifiedKFold(n_splits=5, shuffle=True, random_state=42)

for fold, (train_idx, test_idx) in enumerate(skf.split(X, y)):
    y_train, y_test = y[train_idx], y[test_idx]
    print(f"Fold {fold + 1}:")
    print(f" Train class distribution: {np.bincount(y_train)}")
    print(f" Test class distribution: {np.bincount(y_test)}")
...
```

```
**Output:**
...
```

Fold 1:

Train class distribution: [720 80] # 90% class 0, 10% class 1

Test class distribution: [180 20] # Same ratio!

Fold 2:

Train class distribution: [720 80]

Test class distribution: [180 20]

... (all folds maintain the 90:10 ratio)

```
...
```

### \*\*Key Observation:\*\*

- Each fold's test set has **exactly 10% defaults**, just like the original data.
- Without stratification, some folds might randomly get **0 defaults** or **too many**, leading to biased evaluation.

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### #### \*\*Step 3: Train a Model with Stratified K-Fold\*\*

Let's use Logistic Regression and evaluate accuracy across folds.

```
```python
from sklearn.linear_model import LogisticRegression
from sklearn.metrics import accuracy_score
```

```

model = LogisticRegression()
accuracies = []

for train_idx, test_idx in skf.split(X, y):
    X_train, X_test = X[train_idx], X[test_idx]
    y_train, y_test = y[train_idx], y[test_idx]

    model.fit(X_train, y_train)
    y_pred = model.predict(X_test)
    acc = accuracy_score(y_test, y_pred)
    accuracies.append(acc)
    print(f"Accuracy: {acc:.2f}")

print(f"\nAverage accuracy: {np.mean(accuracies):.2f}")
...

```

**\*\*Output:\*\***  
...

```

Accuracy: 0.92
Accuracy: 0.91
Accuracy: 0.93
Accuracy: 0.90
Accuracy: 0.92

```

```

Average accuracy: 0.92
...

```

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### ### **\*\*Comparison: Stratified vs. Random K-Fold\*\***

#### #### **\*\*Problem with Random K-Fold (No Stratification)\*\***

```

```python
from sklearn.model_selection import KFold

kf = KFold(n_splits=5, shuffle=True, random_state=42)

for fold, (train_idx, test_idx) in enumerate(kf.split(X)):
    y_test = y[test_idx]
    print(f"Fold {fold + 1} test classes: {np.bincount(y_test)}")
...

```

#### **\*\*Possible Output (Unreliable Splits):\*\***

```

...
Fold 1 test classes: [183 17] # 8.5% defaults (close, but not exact)
Fold 2 test classes: [177 23] # 11.5% defaults (oversampled)
Fold 3 test classes: [195 5] # 2.5% defaults (too few!)
...
...

```

### **\*\*Issue:\*\***

- Fold 3 has **\*\*only 5 defaults\*\*** (too few for reliable evaluation).
- Model performance would vary wildly across folds.

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### **### \*\*When Should You Use Stratified K-Fold?\*\***

1. **\*\*Classification Problems\*\*** (especially imbalanced datasets).
2. **\*\*Small Datasets\*\*** (where random splits might miss minority classes).
3. **\*\*Reliable Evaluation\*\*** (when you need consistent class ratios in each fold).

### **\*\*Avoid it for:\*\***

- Regression problems (no classes to stratify).
- Perfectly balanced datasets (normal K-Fold is fine).

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### **### \*\*Final Summary\*\***

- **\*\*Stratified K-Fold = Fair Splitting\*\*** (maintains class ratios).
- **\*\*Normal K-Fold = Random Splitting\*\*** (risks skewed evaluation).
- **\*\*Use Case:\*\*** Fraud detection, medical diagnosis, or any imbalanced classification.

Stratified K-Fold is indeed a powerful tool, especially when dealing with real-world "messy" data where classes are imbalanced. Let me add a few more intuitive insights and a bonus practical scenario to really cement the concept.

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### **### \*\*Bonus: The "Hospital Lab Test" Analogy\*\***

**Imagine you're a researcher testing a new disease-detection AI:**

- Your hospital has **\*\*1,000 patient blood samples\*\***:
  - **\*\*950 healthy\*\*** (class 0)
  - **\*\*50 with a rare disease\*\*** (class 1)

If you split the data randomly into 5 folds (like normal K-Fold), you might accidentally put:

- **\*\*All 50 disease cases into just 1-2 folds\*\*** (other folds get 0 disease cases!)
- Your AI would seem "perfect" in folds with no disease cases (predicting "healthy" every time), but this is dangerously misleading.

**\*\*Stratified K-Fold acts like a careful lab technician:\*\***

- It ensures every fold gets exactly **\*\*10 disease cases\*\*** (5% of each fold, matching the original 5% disease rate).
- Now when your AI scores 95% accuracy, you know it's truly because it works



—not because it lucked out on easy folds.

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### ### **\*\*Advanced Practical Tip: Stratification with Multiple Classes\*\***

What if you have **\*\*3+ classes\*\*** (e.g., "healthy", "mild disease", "severe disease")? Stratified K-Fold handles this too!

```
```python
# Dataset with 3 imbalanced classes (70%, 20%, 10%)
X, y = make_classification(
    n_samples=1000, n_classes=3,
    weights=[0.7, 0.2, 0.1], random_state=42
)

skf = StratifiedKFold(n_splits=5)
for train_idx, test_idx in skf.split(X, y):
    print("Test fold classes:", np.bincount(y[test_idx]))
...

**Output (each fold maintains 70:20:10 ratio):**
...

Test fold classes: [140  40  20] # 70% / 20% / 10%
Test fold classes: [140  40  20]
...
...
```
```

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### ### **\*\*When Stratification Can't Help\*\***

While stratification fixes class imbalance, it **\*\*won't\*\*** help with:

**1. **\*\*Small datasets with tiny minorities\*\***** (e.g., 1,000 samples but only 5 fraud cases → each fold gets just 1 fraud case, which is too few to learn from).

- **\*Solution:** Oversample minority class or use synthetic data (SMOTE).

**2. **\*\*Time-series data\*\***** (where order matters, and random splitting leaks future data into past training).

- **\*Solution:** Use ``TimeSeriesSplit`` instead.

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### ### **\*\*Key Takeaways\*\***

1. **\*\*Stratified K-Fold = "Fair Exam Proctor"\*\***

- Ensures every test fold reflects real-world class ratios.

2. **\*\*Use it by default for classification\*\*** (unless you have a specific reason not to).

3. **Watch out for:**

- Extremely rare classes (may need synthetic data).
- Non-classification problems (e.g., regression).

## ### **LOCO (Leave-One-Covariate-Out) Validation Explained Intuitively**

**LOCO** is a model-agnostic interpretability method that tests how much a **specific feature** impacts your model's predictions—by systematically removing it and measuring the change in performance.

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### ### **Simple Analogy: The "Apple Pie Recipe" Test**

Imagine you're judging an apple pie contest where each pie uses:

- Apples (A)
- Cinnamon (B)
- Sugar (C)

To determine **how critical cinnamon (B) is** to the pie's taste:

1. **Bake a normal pie** (with A+B+C) → Score: 9/10
2. **Remove cinnamon (B)** → New pie (A+C) → Score drops to 6/10
3. **Conclusion**: Cinnamon contributes **+3 points** to the score.

This is exactly how LOCO works for machine learning features!

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### ### **How LOCO Works (Step-by-Step)**

1. **Train your model** on all features (e.g., `[Age, Income, Debt]`).
2. **Remove one feature at a time** (e.g., drop `Income`).
3. **Retrain the model** and measure performance change (e.g., accuracy drop).
4. **Large performance drop?** → That feature was important!

```
```python
```

```
from sklearn.ensemble import RandomForestClassifier
from sklearn.metrics import accuracy_score
```

```
# Original model (all features)
```

```
model_all = RandomForestClassifier().fit(X_train, y_train)
```

```
baseline_acc = accuracy_score(y_test, model_all.predict(X_test))
```

```
# LOCO for 'Income' feature
```

```

X_train_remove = X_train.drop(columns=['Income'])
X_test_remove = X_test.drop(columns=['Income'])

model_remove = RandomForestClassifier().fit(X_train_remove, y_train)
new_acc = accuracy_score(y_test, model_remove.predict(X_test_remove))

print(f"Baseline Accuracy: {baseline_acc:.2f}")
print(f"Accuracy without 'Income': {new_acc:.2f}")
print(f"Importance of 'Income': {baseline_acc - new_acc:.2f}")
` ``

```

## **\*\*Output\*\*:**

```

` ``
Baseline Accuracy: 0.89
Accuracy without 'Income': 0.82
Importance of 'Income': 0.07 # Big drop → Income is critical!
` ``

```

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## **### \*\*Key Use Cases for LOCO\*\***

1. **\*\*Feature Importance Ranking\*\***
  - Find which features *actually* impact predictions (vs. correlation plots).
2. **\*\*Debugging Bias\*\***
  - E.g., If removing `Gender` drops accuracy, your model may be unfairly using it.
3. **\*\*Model Simplification\*\***
  - Identify redundant features (no performance drop when removed).

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## **### \*\*LOCO vs. SHAP/LIME\*\***

Method	Pros	Cons
<b>**LOCO**</b>	Simple, easy to implement	Slow (retrains model for each feature)
<b>**SHAP**</b>	Theoretical guarantees	Computationally expensive
<b>**LIME**</b>	Works for any model	Local explanations only

## **\*\*Rule of Thumb\*\*:**

- Use **\*\*LOCO\*\*** for a quick global importance check.
- Use **\*\*SHAP/LIME\*\*** for detailed local explanations.

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### ### **\*\*When to Avoid LOCO\*\***

- **\*\*High-dimensional data\*\*** (1000+ features → retraining 1000 models is impractical).
- **\*\*Feature interactions\*\*** (LOCO may underestimate importance if features depend on each other).

**\*\*Alternative\*\***: For high-dimensional data, use permutation importance (similar idea but faster).

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### ### **\*\*Try It Yourself!\*\***

Pick a Kaggle dataset (e.g., Titanic survival prediction) and:

1. Train a baseline model.
2. Apply LOCO to columns like `Age`, `Fare`, or `Sex`.
3. See which feature removal hurts accuracy the most!

## **AUC-ROC (Area Under the Receiver Operating Characteristic Curve)**

- **Definition**: AUC measures the ability of the model to distinguish between classes. The ROC curve is a plot of **True Positive Rate (Recall)** vs **False Positive Rate**.
- **Use**:
  - **AUC = 1**: Perfect model.
  - **AUC = 0.5**: No better than random guessing.
  - **AUC > 0.5**: Better than random, but not perfect.

## **Quick Summary on Evaluation:**

- **Accuracy**: Overall correctness of the model.
- **Precision**: Correctness of positive predictions.
- **Recall**: Ability to find all positive cases.
- **F1 Score**: Balance between precision and recall.
- **AUC-ROC**: Measures the model's ability to separate classes.

These metrics provide different insights into model performance, especially when the dataset is imbalanced or when certain types of errors are more costly.

## **Bias vs Variance:**

- **Bias**: Error due to wrong assumptions.
- **Variance**: Error due to model sensitivity to small changes in data.
-

## ✅ Correct Understanding:

Type	Bias	Variance	Description
<b>Underfitting</b>	High bias	Low variance	Model is too simple, misses patterns
<b>Overfitting</b>	Low bias	High variance	Model is too complex, memorizes noise

🧠 So:

- ✅ **High variance** → Model changes a lot with different data → **Overfitting**
- ✅ **Low variance** → Model is stable → May still **underfit** if it has high bias

## 🔄 Common “Wrong Assumptions” in High Bias Models:

Assumption Type	Reality	Impact
Linear relationship	Non-linear patterns	Misses patterns
Few features matter	Many features influence outcome	Poor predictions
Data is clean and balanced	Data is noisy or imbalanced	Misleading results

## Unsupervised Algorithms

Task	Algorithm Examples
<b>Clustering:</b> Group similar data points together.	K-Means, DBSCAN, Hierarchical
<b>Dimensionality Reduction:</b> Reduce the number of features while keeping important info.	PCA, t-SNE, Autoencoders
<b>Association Mining/Association Rule Learning:</b> Find interesting relationships (rules) between items in large datasets.	Apriori

# METRICS FOR EVALUATING MACHINE LEARNING MODELS

## Regressions

- MSE
- MAE
- R Square
- Adjusted R Square

## Classifications

- ROC-AUC
- Log -Loss
- Confusion Metrics

## Unsupervised Models

- Rand Index
- Mutual Information
- Dunn's Index
- Silhouette Coefficient

## Others

- CV Error
- Heuristic methods to find K
- BLEU Score(NLP)



## ◆ 1. Classification Metrics

Used when predicting **categories/labels** (e.g., spam vs. not spam).



### Accuracy

- **Definition:** Correct predictions / Total predictions
- **Use When:** Classes are balanced.



### Precision

- **Definition:** True Positives / (True Positives + False Positives)
- **Use When:** False positives are costly (e.g., email spam filter).



### Recall (Sensitivity / True Positive Rate)

- **Definition:** True Positives / (True Positives + False Negatives)
- **Use When:** False negatives are costly (e.g., disease detection).



### F1-Score

- **Definition:** Harmonic mean of precision and recall
- **Use When:** You want a balance between precision and recall.



### Confusion Matrix

- **Definition:** A table showing TP, TN, FP, FN
- **Use:** Gives a detailed view of model performance.

### **ROC Curve & AUC**

- **ROC Curve:** Plots TPR vs. FPR
- **AUC:** Area under the ROC curve; closer to 1 is better.

## **2. Regression Metrics**

Used when predicting **continuous values** (e.g., house price prediction).

### **Mean Absolute Error (MAE)**

- **Definition:** Average of absolute differences between predicted and actual values
- **Pros:** Easy to understand; less sensitive to outliers.

### **Mean Squared Error (MSE)**

- **Definition:** Average of squared differences between predicted and actual values
- **Pros:** Penalizes large errors more than MAE.

### **Root Mean Squared Error (RMSE)**

- **Definition:** Square root of MSE
- **Pros:** Same unit as target variable.

### **R<sup>2</sup> Score (Coefficient of Determination)**

- **Definition:** Proportion of variance explained by the model
- **Range:**  $-\infty$  to 1 (1 = perfect prediction)

## **Evaluation Metrics:**

**Classification:**

- **Accuracy** =  $(TP + TN) / \text{Total}$
- **Precision** =  $TP / (TP + FP)$  → How many predicted positives were correct
- **Recall** =  $TP / (TP + FN)$  → How many actual positives were identified
- **F1-score** =  $2 * (\text{Precision} * \text{Recall}) / (\text{Precision} + \text{Recall})$

**Regression:**

- **MAE:** Mean Absolute Error
- **MSE:** Mean Squared Error
- **RMSE:** Root Mean Squared Error
- **R<sup>2</sup> score:** Percentage of variance explained by the model

## **Evaluation Metrics**

### **For Classification Models**

Metric	Formula	Description
--------	---------	-------------

<b>Accuracy</b>	$(TP + TN) / (TP + TN + FP + FN)$	Measures overall correctness. Use when classes are balanced.
<b>Precision</b>	$TP / (TP + FP)$	Out of all predicted positives, how many are correct. Use when <b>false positives</b> are costly (e.g., spam detection).
<b>Recall</b>	$TP / (TP + FN)$	Out of all actual positives, how many were identified. Use when <b>false negatives</b> are costly (e.g., cancer detection).
<b>F1-score</b>	$2 \times (Precision \times Recall) / (Precision + Recall)$	Harmonic mean of precision and recall. Best when you need balance between precision and recall.

💡 **Example (Confusion Matrix):**

	<b>Predicted Positive</b>	<b>Predicted Negative</b>
Actual Positive	TP	FN
Actual Negative	FP	TN

📈 **For Regression Models**

<b>Metric</b>	<b>Description</b>
<b>MAE (Mean Absolute Error)</b>	Average of absolute errors: $\text{mean}( \text{actual} - \text{predicted} )$
<b>MSE (Mean Squared Error)</b>	Average of squared errors: $\text{mean}((\text{actual} - \text{predicted})^2)$ ♦ Penalizes large errors more (good if large errors are bad).
<b>RMSE (Root Mean Squared Error)</b>	Square root of MSE: $\sqrt{\text{MSE}}$ ♦ In the same unit as the original data.
<b>R<sup>2</sup> Score (R-squared)</b>	<b><math>1 - (SS_{\text{res}} / SS_{\text{total}})</math></b> ♦ Explains how well the model explains variance in the data. ♦ Ranges from 0 to 1 (closer to 1 is better).