# Introduction to Machine Learning

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# Definition of Machine Learning



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# Definition of Machine Learning

## General definition

Machine Learning enables computers to learn from data without explicit programming

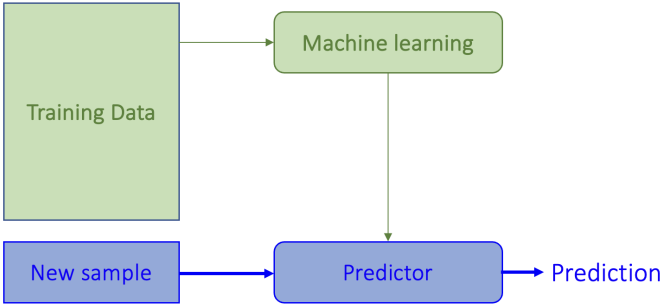


**Figure 1.1**

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# Definition of Machine Learning

## Mitchell, 1997

- A computer program learns if its performance (P) at some task (T) improves with experience (E)
- Three components:
  1. T: Task
  2. P: Performance metric
  3. E: Experience

## Example

- Task, Predictor:
  - Task = email classification
  - Predictor = email classifier
- Data Training, Experience: Labeled emails
- Performance: Accuracy, Precision, Recall, F1-Score, etc.

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# Traditional Methods vs Machine Learning

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# Traditional Methods vs Machine Learning

| | **Traditional Methods** (Rule-based / Explicit Programming) | **Machine Learning** |
|---|---|---|
| **Approach** | Rules are explicitly coded by humans | Learns patterns automatically from data |
| **Knowledge Source** | Human expert knowledge | Data (experience) |
| **Flexibility** | Hard to scale, brittle with complex tasks | Adapts to new data and tasks |
| **Performance** | Depends on the quality of hand-written rules | Improves with more data and training |
| **Examples** | Expert systems, calculators, deterministic algorithms | Image recognition, speech recognition, spam filtering |

**Difference**

- Traditional = rules by humans
- ML = rules learned from data


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# Types of Machine Learning

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# Types of Machine Learning

## Supervised Learning

- Learn from **labeled data**: Input $\rightarrow$ Output
- Goal: predict output for new unseen data
- **Typical Tasks**:
  - Regression: predict continuous values (e.g., house price)
  - Classification: assign labels (e.g., spam vs. not spam)
  - Detection: locate objects in images (e.g., face detection)
  - Identification: recognize entities (e.g., speaker ID, person re-ID)
  - Others: segmentation, time-series forecasting, recommendation

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# Types of Machine Learning

## Unsupervised Learning

- Learn from **unlabeled data**: Input only (no output labels)
- Goal: discover hidden structure / representations
- **Typical Tasks**:
  - Clustering: group similar data (e.g., customer segmentation)
  - Dimensionality Reduction: compress features (e.g., PCA, t-SNE, UMAP)
  - Density Estimation: model $p(x)$ (e.g., Gaussian Mixture Models)
  - Anomaly/Outlier Detection: find rare or abnormal patterns
  - Topic Modeling: uncover latent topics in documents (e.g., LDA)
  - Representation Learning: learn embeddings/features (e.g., autoencoders)

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# Types of Machine Learning

## Reinforcement Learning

- Learn by **interacting with an environment**.
- Agent receives **state** $s$, takes an **action** $a$, and gets a **reward** $r$.
- Goal: learn a policy $\pi(a|s)$ that maximizes **cumulative reward**.
- **Typical Tasks**:
  - Game Playing: Chess, Go, Atari, AlphaZero
  - Robotics: motion control, grasping
  - Resource Allocation: scheduling, network optimization
  - Recommendation Systems: adaptively suggest content
  - Autonomous Driving: decision-making in dynamic environments

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# Components of a Machine Learning System

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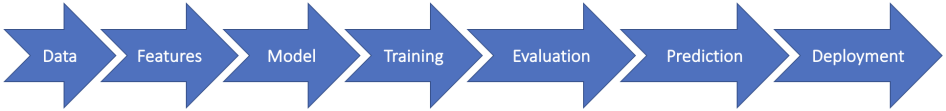
# Components of a Machine Learning System




1. **Data:**
   - Raw data collected from various sources.
   - Includes training data, validation data, and test data (iid principle)
2. **Features:**
   - Relevant variables (features) extracted from raw data.
   - Feature engineering & feature selection are critical steps.
   - In deep learning: features are learnt from raw data.

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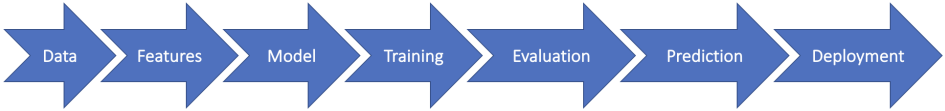
# Components of a Machine Learning System




### ❸ Model:

- Algorithm or architecture used to learn patterns from data.
- Examples: Linear Regression, Decision Tree, Neural Networks.

### ❹ Training:

- Process of feeding data into the model to adjust parameters.
- Requires optimization (e.g., gradient descent).

### ❺ Evaluation:

- Assess model performance using metrics (accuracy, precision, recall, F1, etc.).
- Prevent overfitting via validation.

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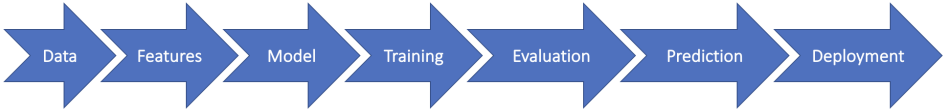
# Components of a Machine Learning System




**6 Prediction/Inference:**

- Apply the trained model to unseen data.
- Output results such as classification, regression, recommendations.

**7 Deployment & Monitoring (optional but practical):**

- Model integration into real-world systems.
- Continuous monitoring & updating as new data arrives.

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# Phases in the Machine Learning Process



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# Phases in the Machine Learning Process

1. **Problem Definition**
   - Define task, objectives, and success metrics.
2. **Data Collection**
   - Gather raw data from multiple sources.
3. **Data Preprocessing**
   - Clean, normalize, handle missing values.
   - Split into training, validation, test sets.
4. **Feature Engineering**
   - Extract and select relevant features.
   - Transform raw data into useful representations.

# Phases in the Machine Learning Process

### ❺ Model Selection & Training
- Choose suitable algorithm/architecture.
- Train model using training data.

### ❻ Model Evaluation
- Validate on unseen data.
- Metrics: accuracy, precision, recall, F1, etc.

### ❼ Deployment
- Integrate model into real-world applications.

### ❽ Monitoring & Maintenance
- Track performance over time.
- Retrain with new data if needed.

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# Performance Metrics & Model Evaluation

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# Performance Metrics & Model Evaluation


## Performance Metrics (Formulas in Section "Performance Metrics:Detail")

- **Classification**: Accuracy, Precision, Recall, F1-Score, ROC-AUC.
- **Regression**: MSE (Mean Squared Error), RMSE, MAE, $R^2$.
- **Ranking / Retrieval**: Precision@k, Recall@k, MAP (Mean Average Precision), NDCG.

## Consideration

- Choose metrics that align with the task (e.g., F1 for imbalanced data).
- Avoid overfitting: compare training vs validation/test results.
- Monitor performance drift after deployment.

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# Performance Metrics & Model Evaluation

## Model Evaluation Techniques

- **Hold-out**: Split into training, validation, and test sets.
- **Cross-validation (k-fold)**: Robust evaluation with multiple splits.
- **Bootstrap**: Resampling-based evaluation.

## Consideration

- Ensure data splits are representative (avoid leakage).
- Use cross-validation for small datasets to improve robustness.
- Be mindful of computation cost when using k-fold or bootstrap.
- Always keep a final unseen test set for unbiased evaluation.

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# Training, Validation, and Test Sets

## Data Splits

- **Training set**: Used to fit model parameters.
- **Validation set**: Used for hyperparameter tuning and model selection.
- **Test set**: Used only once for final unbiased evaluation.

## Principles

- Data should be split under the **i.i.d assumption** (independent and identically distributed).
- **No information leakage between training and test sets.**
- Typical split: 70% train, 15% validation, 15% test (but depends on dataset size).

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# k-Fold Cross Validation


## Idea

- Split dataset into $k$ equally sized folds.
- Train on $k-1$ folds and validate on the remaining fold.
- Repeat $k$ times, each fold serving as validation once.
- Average the evaluation metrics across all folds.

## Final Step

- After model selection, retrain the chosen model on the **entire dataset**.
- Ensures best use of available data for deployment.

## Benefit

- Every sample is used for both training and validation.
- Provides a more reliable estimate of model performance.

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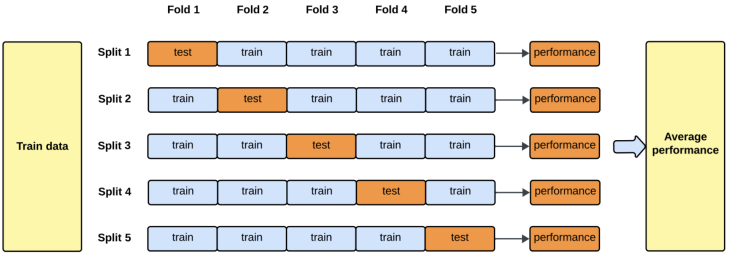
# k-Fold Cross Validation: Illustration




- Example: $k = 5$ folds.
- Each fold rotates as the test set.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# Bootstrap Evaluation

## Idea

- Resample the dataset **with replacement** to create many bootstrap samples (each of size $n$).
- Train a model on each bootstrap sample and evaluate its performance.
- Aggregate the results to estimate performance and uncertainty.

## Procedure

- Repeat for $B$ bootstrap iterations ($B$=100$\sim$1000):
  - Draw a bootstrap sample of size $n$ from the original data.
  - Fit the model on the bootstrap sample.
  - Evaluate using out-of-bag (OOB) data or an internal validation split.

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# Bootstrap: Estimation and OOB

## Aggregating Metrics

- Report the **mean** and **standard deviation** of metrics across $B$ runs.
- Construct **confidence intervals** (e.g., percentile CI from the empirical distribution).

## Out-of-Bag (OOB) Evaluation

- On average, about 36.8% [1] of samples are not included in a bootstrap draw.
- Use these OOB samples as a natural validation set for each bootstrap model.

[1] $n$: number of samples. OOB probabity: $\left(1 - \frac{1}{n}\right)^n \approx e^{-1} \approx 0.368$

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# Bootstrap: Considerations and Final Model

## Considerations

- Resampling with replacement may duplicate some points and omit others.
- Useful for small datasets and for estimating uncertainty (variance of metrics).
- Variants: **.632 bootstrap** mixes in OOB error to reduce bias.

## Final Step

- After model/hyperparameter selection, **retrain the chosen model on the entire dataset**.
- This maximizes data usage for deployment.

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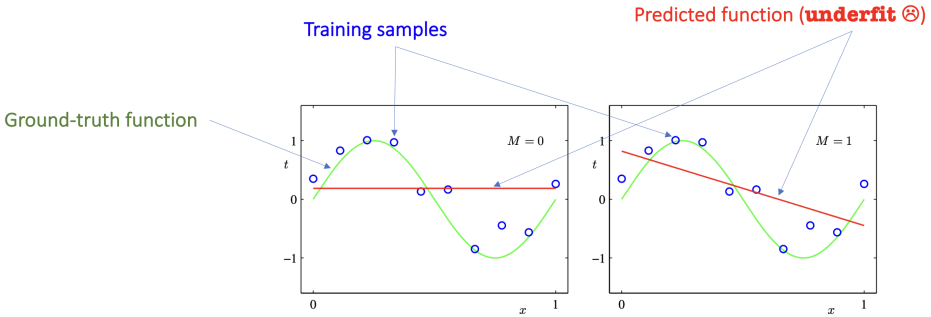
# Overfitting, Underfitting, and Good-fit

## Underfitting

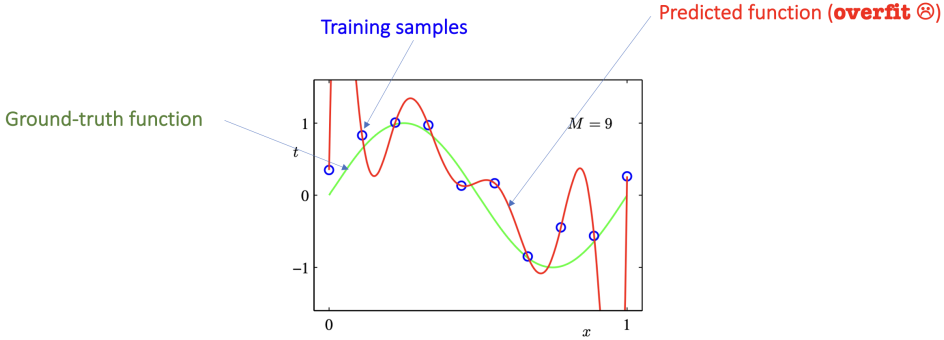
- Model too simple → fails to capture patterns.
- **High training error & high test error.**



# Overfitting, Underfitting, and Good-fit

## Overfitting

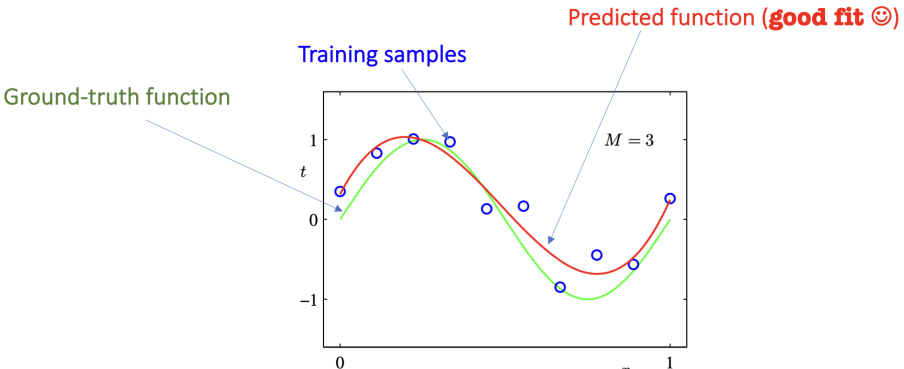
- Model too complex → memorizes noise.
- **Low training error but high test error.**



# Overfitting, Underfitting, and Good-fit

## Good Fit (Right Complexity)

- Model captures the underlying patterns without memorizing noise. item Balanced training and test errors. item Achieves good generalization on unseen data.



# The Bias–Variance Trade-off



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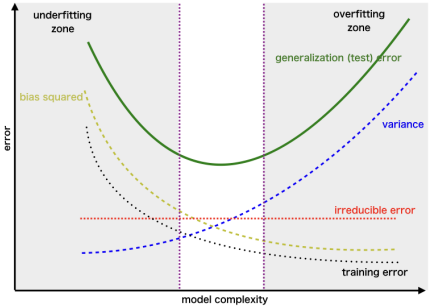
# The Bias–Variance Trade-off

## Concepts

- **Bias**: Error due to overly simple models, failing to capture underlying patterns. ($\rightarrow$ Underfitting)
- **Variance**: Error due to overly complex models, sensitive to noise and small changes. ($\rightarrow$ Overfitting)
- Goal: Find the balance (trade-off) for a **good fit**.

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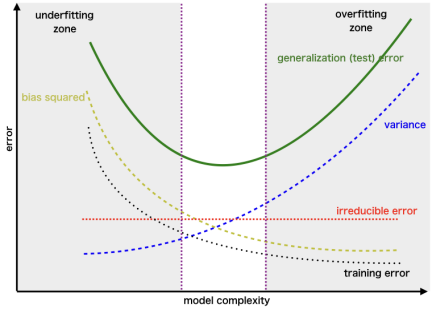
# The Bias–Variance Trade-off

## Practical Implications

- **High bias** → use more complex models, add features.
- **High variance** → apply regularization, collect more data, reduce dimensionality.
- Use cross-validation to identify the sweet spot.



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# Bias–Variance Decomposition

## Error Components

The expected squared error can be decomposed into three parts:

$$\mathbb{E}\big[(y - \hat{f}(x))^2\big] = \underbrace{(\mathbb{E}[\hat{f}(x)] - f(x))^2}_{\text{Bias}^2} + \underbrace{\mathbb{E}\big[(\hat{f}(x) - \mathbb{E}[\hat{f}(x)])^2\big]}_{\text{Variance}} + \underbrace{\sigma^2}_{\text{Noise}}$$

- **Bias**$^2$: Error due to model's inability to represent the true function (underfitting).
- **Variance**: Error from sensitivity to training data (overfitting).
- **Noise**: Irreducible error caused by randomness or measurement noise in data.

- Read "**Bias–Variance: Derivation**" for detail information.

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# Generalization and the Importance of Data



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# Generalization and the Importance of Data

## Generalization

- The true goal of machine learning is not to memorize training data, but to generalize to unseen data.
- A well-generalized model balances bias and variance, achieving strong performance on both training and test sets.
- Overfitting reduces generalization by tailoring too closely to training examples.



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# Generalization and the Importance of Data

## The Role of Data

- More high-quality and diverse data usually improves generalization.
- Data preprocessing (cleaning, normalization, augmentation) is as important as model choice.
- Imbalanced or biased data leads to poor generalization, even with powerful models.
- The diversity of training data determines how well the model performs in the real world.

## Key Message

Generalization depends not only on the algorithm but also heavily on the quality, diversity, and representativeness of the data.



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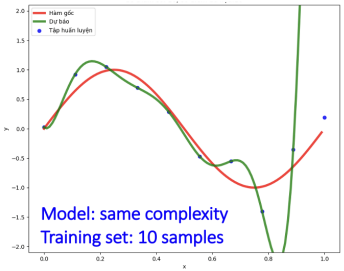


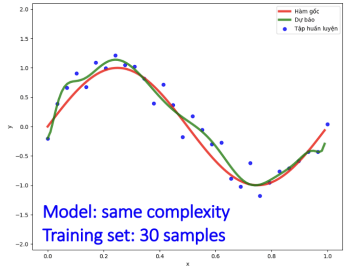


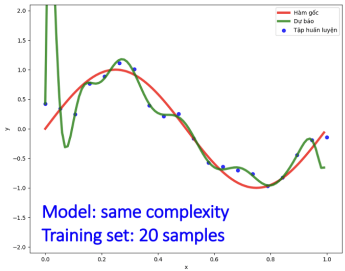


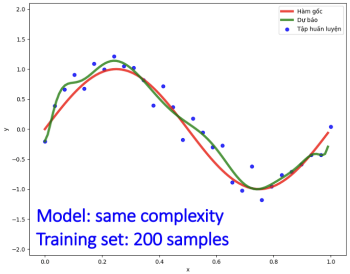




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# Generalization and the Importance of Data



**Key Idea**

- With the same model complexity, **more training data** leads to better generalization.
- Small datasets cause the model to overfit noise (high variance).
- Larger datasets allow the model to capture the true underlying function.

**Takeaway**

More data $\Rightarrow$ smoother predictions, less overfitting, and improved generalization performance.

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# Performance Metrics: Detail



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# Classification Metrics: Two-Class

## Confusion Matrix Terms

| | Predicted Positive | Predicted Negative |
|---|---|---|
| Actual Positive | $TP$ | $FN$ |
| Actual Negative | $FP$ | $TN$ |

## Formulas

- Accuracy $= \dfrac{TP + TN}{TP + TN + FP + FN}$
- Precision $= \dfrac{TP}{TP + FP}$
- Recall $= \dfrac{TP}{TP + FN}$

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# Classification Metrics: Two-Class

## Confusion Matrix Terms

| | Predicted Positive | Predicted Negative |
|---|---|---|
| Actual Positive | *TP* | *FN* |
| Actual Negative | *FP* | *TN* |

## Formulas

- F1-Score $= 2 \cdot \dfrac{\text{Precision} \cdot \text{Recall}}{\text{Precision} + \text{Recall}}$
- ROC-AUC = Area under ROC curve (TPR vs FPR)

# Classification Metrics: Multi-Class

## Confusion matrix

$$C = \begin{bmatrix} c_{11} & c_{12} & \dots & c_{1K} \\ c_{21} & c_{22} & \dots & c_{2K} \\ \vdots & \vdots & \ddots & \vdots \\ c_{K1} & c_{K2} & \dots & c_{KK} \end{bmatrix}$$

- $c_{ij}$: number of samples of true class $i$ predicted as class $j$.
- Row sum $\sum_j c_{ij}$ = number of samples in class $i$ (ground truth).
- Column sum $\sum_i c_{ij}$ = number of predictions in class $j$.
- Diagonal sum $\sum_k c_{kk}$ = correctly classified samples.
- Total samples $N = \sum_{i,j} c_{ij}$.

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# Classification Metrics: Multi-Class

$$\text{Accuracy} = \frac{\sum_{k=1}^{K} c_{kk}}{N}$$

For each class $k$:

$$\text{Precision}_k = \frac{c_{kk}}{\sum_i c_{ik}}, \quad \text{Recall}_k = \frac{c_{kk}}{\sum_j c_{kj}}$$

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

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# Classification Metrics: Multi-Class

$$\text{Macro-Precision} = \frac{1}{K}\sum_{k=1}^{K}\text{Precision}_k$$

$$\text{Macro-Recall} = \frac{1}{K}\sum_{k=1}^{K}\text{Recall}_k$$

$$\text{Macro-F1} = \frac{1}{K}\sum_{k=1}^{K}\text{F1}_k$$

- Treats all classes equally, regardless of their size.
- Useful when class imbalance exists and each class is equally important.

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# Classification Metrics: Multi-Class

$$\text{Weighted-Precision} = \sum_{k=1}^{K} w_k \cdot \text{Precision}_k, \quad w_k = \frac{n_k}{N}$$

$$\text{Weighted-Recall} = \sum_{k=1}^{K} w_k \cdot \text{Recall}_k$$

$$\text{Weighted-F1} = \sum_{k=1}^{K} w_k \cdot \text{F1}_k$$

- $n_k$: number of samples in class $k$.
- $N$: total number of samples.
- Larger classes have stronger influence on the score.



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# Classification Metrics: Multi-Class

$$\text{Micro-Precision} = \frac{\sum_{k=1}^{K} TP_k}{\sum_{k=1}^{K} (TP_k + FP_k)}$$

$$\text{Micro-Recall} = \frac{\sum_{k=1}^{K} TP_k}{\sum_{k=1}^{K} (TP_k + FN_k)}$$

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

- Aggregates contributions of all classes before computing the metric.
- Equivalent to accuracy in multi-class setting.
- For multi-label classification, micro-averaged metrics may differ from accuracy.

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# ROC and AUC: Definitions

## ROC Curve

ROC plots **TPR** vs **FPR** by sweeping a decision threshold on predicted scores.

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

## AUC (Area Under the ROC Curve)

$$\text{AUC} = \int_0^1 \text{TPR}(\text{FPR})\, d(\text{FPR})$$

Equivalent interpretation:

$$\text{AUC} = \mathbb{P}\left(s^+ > s^-\right)$$

where $s^+$ and $s^-$ are scores of random positive and negative samples.

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# ROC-AUC: Computation and Notes

- Sort samples by predicted score; sweep threshold to compute points (FPR, TPR).
- Approximate area with the trapezoidal rule (sklearn does this by default).
- Robust to class-imbalance (uses ranking of scores rather than fixed threshold).
- Multi-class: use one-vs-rest (macro/micro) averaging for ROC-AUC.



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# ROC-AUC in scikit-learn

- ROC curve points:

```
from sklearn.metrics import roc_curve, auc
# y_score: predicted scores for the positive class
# e.g., y_score = clf.predict_proba(X)[:, 1]
# or  clf.decision_function(X)
fpr, tpr, thr = roc_curve(y_true, y_score)
roc_auc = auc(fpr, tpr)
```

- Direct AUC:

```
from sklearn.metrics import roc_auc_score
# Binary:
roc_auc_score(y_true, y_score)

# Multi-class (Y_scores shape: n_samples x n_classes):
roc_auc_score(y_true, Y_scores, multi_class="ovr", average="macro")
```



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# Regression Metrics: Detail




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## Mean Absolute Error (MAE)

Evaluate how well predicted values $\hat{y}$ approximate true values $y$.

$$\text{MAE} = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i|$$

- Measures average magnitude of errors.
- Robust to outliers compared to MSE.

# Regression Metrics: Detail




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## Mean Squared Error (MSE)

Average of squared differences between predicted and true values.

$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

- Penalizes larger errors more heavily than MAE.
- Sensitive to outliers.

# Regression Metrics: Detail



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## Root Mean Squared Error (RMSE)

Square root of MSE, interpretable in the same unit as $y$.

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}$$

- Emphasizes large deviations.
- Useful when error magnitude should be in the same scale as target.

# Regression Metrics: Detail



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## Coefficient of Determination ($R^2$)

Measures proportion of variance in $y$ explained by the model.

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2}$$

- $R^2 = 1$: perfect prediction.
- $R^2 = 0$: no better than predicting the mean.
- $R^2 < 0$: worse than a constant mean model.

# Bias–Variance: Derivation



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# Bias–Variance: Derivation



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We start with the expected squared prediction error:

$$\mathbb{E}\big[(y - \hat{f}(x))^2\big]$$

Here:

- $y = f(x) + \epsilon$, where $f(x)$ is the true function and $\epsilon$ is random noise with $\mathbb{E}[\epsilon] = 0$.
- $\hat{f}(x)$ is the prediction from a learning algorithm trained on a dataset (a random function depending on the sample).

# Bias–Variance: Derivation

Substitute $y = f(x) + \epsilon$:

$$\mathbb{E}\big[(f(x) + \epsilon - \hat{f}(x))^2\big]$$

This expresses the error in terms of the true function $f(x)$, the predictor $\hat{f}(x)$, and the noise $\epsilon$.

# Bias–Variance Trade-off: Derivation

Expand the square:

$$= \mathbb{E}\left[(f(x) - \hat{f}(x))^2\right] + 2\mathbb{E}[(f(x) - \hat{f}(x)) \cdot \epsilon] + \mathbb{E}[\epsilon^2]$$

# Bias–Variance: Derivation

Assume that the noise term $\epsilon$:

- has zero mean: $\mathbb{E}[\epsilon] = 0$,
- is independent of $x$ (and hence independent of $\hat{f}(x)$).

Then the cross-term vanishes:

$$\mathbb{E}[(f(x) - \hat{f}(x)) \cdot \epsilon] = \mathbb{E}[f(x) - \hat{f}(x)] \cdot \mathbb{E}[\epsilon] = 0$$

So the decomposition simplifies to:

$$\mathbb{E}\left[(y - \hat{f}(x))^2\right] = \mathbb{E}\left[(f(x) - \hat{f}(x))^2\right] + \mathbb{E}[\epsilon^2]$$

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# Bias–Variance: Derivation

To decompose the model error term:

$$\mathbb{E}\big[(f(x) - \hat{f}(x))^2\big],$$

we introduce the expected model prediction $\mu(x) = \mathbb{E}[\hat{f}(x)]$.
By adding and subtracting $\mu(x)$, we do not change the value:

$$= \mathbb{E}\big[\big(f(x) - \mu(x) + \mu(x) - \hat{f}(x)\big)^2\big].$$

This trick allows us to separate the error into:

- Bias: $(f(x) - \mu(x))^2$
- Variance: $\mathbb{E}[(\hat{f}(x) - \mu(x))^2]$



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# Bias–Variancef: Derivation

Expanding:

$$= (f(x) - \mathbb{E}[\hat{f}(x)])^2 + \mathbb{E}\big[(\hat{f}(x) - \mathbb{E}[\hat{f}(x)])^2\big]$$

- The first term is the **Bias** squared.
- The second term is the **Variance**.

# Bias–Variance: Derivation

So the total expected squared error is:

$$\mathbb{E}\left[(y - \hat{f}(x))^2\right] = \underbrace{(\mathbb{E}[\hat{f}(x)] - f(x))^2}_{\text{Bias}^2} + \underbrace{\mathbb{E}\left[(\hat{f}(x) - \mathbb{E}[\hat{f}(x)])^2\right]}_{\text{Variance}} + \underbrace{\sigma^2}_{\text{Noise}}$$