CS-470: Machine Learning

Week 1 — Introduction to Machine Learning

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Outline

1. Course Logistics
2. Introduction to Machine Learning
3. Types of Machine Learning
4. Challenges of Machine Learning
5. Summary

Course Logistics

- Weekly lectures accompanied by a programming tutorial session
- Assessments include assignments, quizzes, a mid-semester exam, and a final exam
- Strongly encouraged to complete the Coursera *Machine Learning Specialization* by Andrew Ng

Week-01 Python Tutorials

- A Python tutorial notebook has been provided on the course LMS
- Covers basic Python concepts and syntax
- Intended for hands-on practice alongside lectures
- Please download the notebook and complete the exercises
- Bring any questions to the next class for discussion

Evaluation Criteria

Tentative

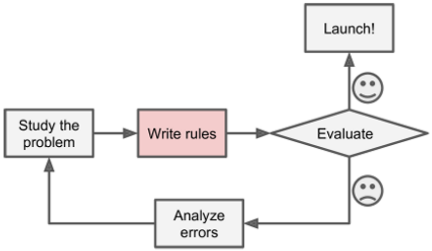
- Assignments: 20%
- Quizzes: 10%
- Midterm: 30%
- Final: 40%

What is Machine Learning?

- Field of study that gives computers the ability to learn without being explicitly programmed. —Arthur Samuel, 1959.
- Focuses on building models that generalize from data
- A computer program is said to learn from experience E with respect to some task T and some performance measure P, if its performance on T, as measured by P, improves with experience E. —Tom Mitchell, 1997.

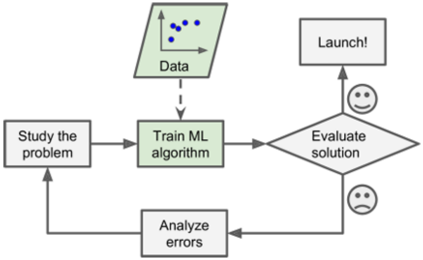
Traditional vs Machine Learning Approach

Traditional Programming



- Hand-coded logic
- Works well for deterministic tasks

Machine Learning



- Learns patterns automatically
- Works well for complex tasks

Source: A. Géron, Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow (O'Reilly).

When to Use Machine Learning?

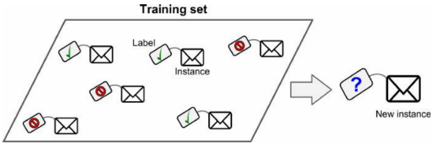
- Tasks where traditional solutions need extensive hand-tuning or rule lists (e.g., spam email filtering)
- Complex problems with no effective traditional solution (e.g., speech recognition)
- Dynamic or changing environments where systems must adapt to new data
- Extracting insights from complex problems or large datasets

Real-World Applications

- Email spam filtering
- Recommendation systems (Netflix, YouTube)
- Medical diagnosis and drug discovery
- Self-driving cars

Supervised Learning

- In supervised learning, training data includes the correct answers, called *labels*.
- Types of supervised algorithms include
    - k-Nearest Neighbors
    - Linear Regression
    - Logistic Regression
    - Support Vector Machines (SVMs)
    - Decision Trees and Random Forests
    - Neural networks



Classification vs Regression

Classification

- Predicts **discrete categories/classes**
- Output is a **label**
- Examples:
  - Spam vs Not Spam
  - Cat vs Dog image
  - Disease: Positive vs Negative
- Evaluation metrics: Accuracy, Precision, Recall, F1-score

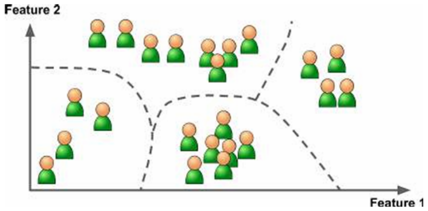
Regression

- Predicts **continuous numeric values**
- Output is a **real number**
- Examples:
  - Predicting house prices
  - Forecasting temperature
  - Predicting stock prices
- Evaluation metrics: MSE, RMSE, MAE, R^2

Both are forms of **Supervised Learning** (learn from labeled data).

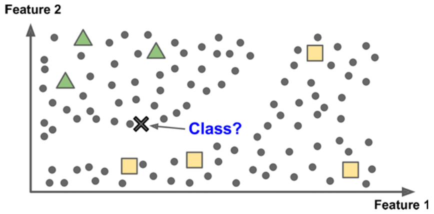
Unsupervised Learning

- In unsupervised learning, the training data is *unlabeled*, and the system learns patterns without guidance.
- Common unsupervised learning algorithms:
  - Clustering
  - Anomaly detection and novelty detection
  - Visualization and dimensionality reduction (PCA, t-SNE)
  - Association rule learning



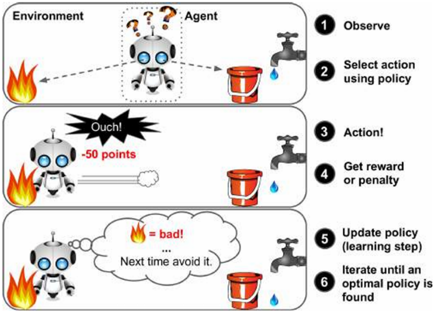
Semi-supervised Learning

- Semi-supervised learning combines aspects of supervised and unsupervised learning.
- A small portion of the data is *labeled*, and the system uses it to automatically label the much larger *unlabeled* portion.
- Common applications include Google Photos and news article categorization.



Reinforcement Learning

- In reinforcement learning, an *agent* interacts with an *environment*, takes actions, and receives *rewards* or *penalties* as feedback.
- The agent learns an optimal *policy*, which is a strategy for choosing actions that maximizes the total reward over time.


Environment
Agent
Ouch!
-50 points
= bad!
...
Next time avoid it.
1 Observe
2 Select action using policy
3 Action!
4 Get reward or penalty
5 Update policy (learning step)
6 Iterate until an optimal policy is found

Example Datasets

- Supervised: Housing prices, image classification
- Unsupervised: Customer segmentation, clustering news articles
- Reinforcement: Game playing, robotic control

Insufficient Quantity of Training Data

- Machine learning models need large amounts of data for effective training.
- Simple tasks may require thousands of examples, while complex tasks (e.g., speech recognition) may need millions.
- A well-known Microsoft study showed that even simple models can achieve strong performance on complex tasks when trained on very large datasets.

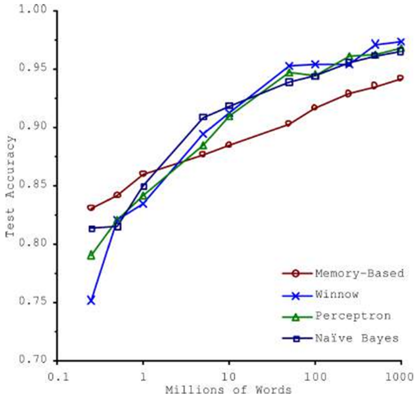


Figure: The importance of Data vs Algorithms

Non-representative Training Data

- To generalize well, training data must reflect the real-world cases we want to predict.
- Non-representative data leads to models that perform poorly on unseen data.
- **Sampling Noise:** Small training sets may miss important patterns and fail to generalize.
- **Sampling Bias:** Even large datasets can be misleading if collected using flawed methods.
- *Example:* In the 1936 U.S. election, a survey by *Literary Digest* predicted a Republican win, but it over-sampled wealthy individuals. Roosevelt (Democrat) won decisively.

Poor-Quality Data

- If training data contains errors, outliers, or noise (e.g., due to poor measurements), the model will struggle to detect underlying patterns and perform well.
- Cleaning and preprocessing data is often time-consuming but crucial. Most data scientists spend a large part of their time on this step.
- **Handling poor-quality data:**
    - Remove or correct obvious outliers.
    - Handle missing values:
        - Ignore the affected feature altogether.
        - Drop instances with missing values.
        - Fill missing values (e.g., with median or mean).
        - Train separate models with and without the feature.

Irrelevant Features

- As the saying goes: *garbage in, garbage out.*
- A model can only learn well if the training data includes enough **relevant** features and avoids too many **irrelevant** ones.
- Designing a good set of features (**feature engineering**) is critical for ML success.
- **Feature engineering involves:**
  - **Feature selection:** Choosing the most useful existing features.
  - **Feature extraction:** Combining or transforming features (e.g., using dimensionality reduction).
  - **Creating new features:** Collecting or deriving additional data.

Overfitting the Training Data

- **Overfitting:** When a model performs well on training data but fails to generalize to unseen data.
- Happens when the model is **too complex** relative to the size or noisiness of the training set.
- Complex models can pick up on **random noise or irrelevant patterns**, mistaking them for real patterns.
- Root cause: Overgeneralizing from limited or noisy data.

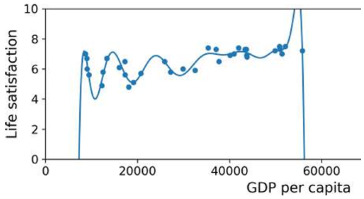


Figure: Overfitting the training data

Preventing Overfitting

- **Simplify the model:**
  - Use fewer parameters (e.g., linear vs high-degree polynomial model)
  - Reduce number of features
  - Apply constraints (regularization)
- **Improve training data:**
  - Collect more data
  - Clean data to remove noise/outliers
- **Regularization:** Adds constraints to keep model weights small
  - Balances fit vs. simplicity
  - Controlled by a **hyperparameter** (set before training)

Underfitting the Training Data

- **Underfitting:** When a model is **too simple** to capture the underlying structure of the data.
- Performs poorly even on the training data (and thus also on new data).
- Example: A simple linear model may underfit if the real relationship is more complex.
- **How to address underfitting:**
  - Use a more powerful model (with more parameters)
  - Provide better features (*feature engineering*)
  - Reduce constraints (e.g., lower regularization)

Testing and Validating Models

- The only way to know how well a model generalizes is to test it on **new data**.
- Deploying directly to production is risky because poor models will impact users.
- Better approach: **split data** into
  - **Training set**: used to train the model
  - **Test set**: used to estimate generalization error (out-of-sample error)
- If training error is low but test error is high, the model is **overfitting**.
- Typical split is **80% training and 20% testing** (depends on dataset size)

Hyperparameter Tuning and Model Selection

- Directly using the test set to pick models can lead to overfitting on the test set
- **Holdout validation:**
    - Split data into training, validation, and test sets
    - Train models with different hyperparameters on training set
    - Select the model that performs best on validation set
    - Retrain the best model on full training data, then evaluate on test set
- **Cross-validation:**
    - Split data into multiple folds
    - Train and evaluate on different folds, average the scores
    - Gives a more reliable performance estimate when data is limited
- Helps choose model type and hyperparameter values while reducing overfitting risk

No Free Lunch Theorem

- Models simplify observations by discarding details unlikely to generalize
- Choosing what to keep/discard requires assumptions about the data
- Example: Linear models assume data is fundamentally linear, and deviations are noise
- **No Free Lunch (NFL) Theorem — David Wolpert (1996):**
  - Without assumptions, no model is better than any other
  - The best model depends on the dataset
  - No single model works best for all problems
- In practice:
  - Make reasonable assumptions about the data
  - Evaluate a few suitable models (e.g., linear models for simple tasks, neural networks for complex tasks)

Summary of Week 1

- Defined Machine Learning and its real-world importance
- Discussed main types of ML: supervised, unsupervised, and reinforcement learning
- Reviewed key ML challenges: data quality, irrelevant features, underfitting, overfitting
- Covered model evaluation: train/validation/test sets, generalization error
- Introduced hyperparameter tuning, model selection, and the No Free Lunch theorem

Takeaway: Strong data, thoughtful model design, and rigorous evaluation are essential for ML success.