

CS 405/605 Data Science

Dr. Qianqian Tong

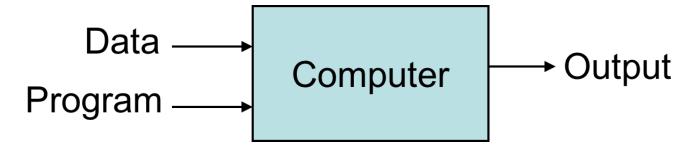
Introduction to ML: agenda

- ML basis
- Linear Regression
- Classification: SVM (kernel)
- Decision Tree & random forest
- Validation
- Dimensionality PCA
- Clustering: Kmeans
- Visualization

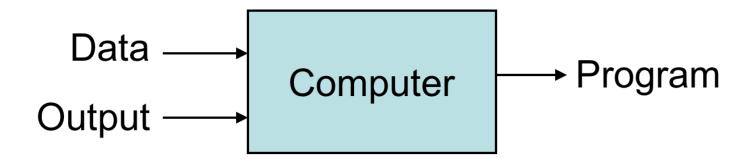




Traditional Programming



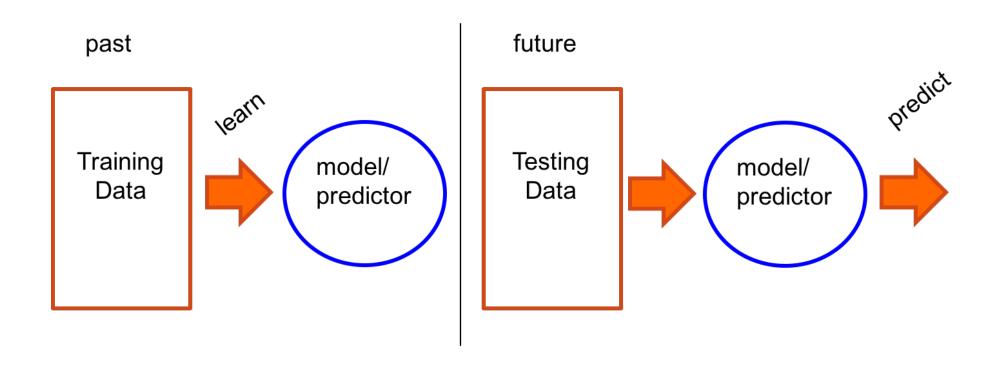
Machine Learning







Machine learning is about predicting the future based on the past.

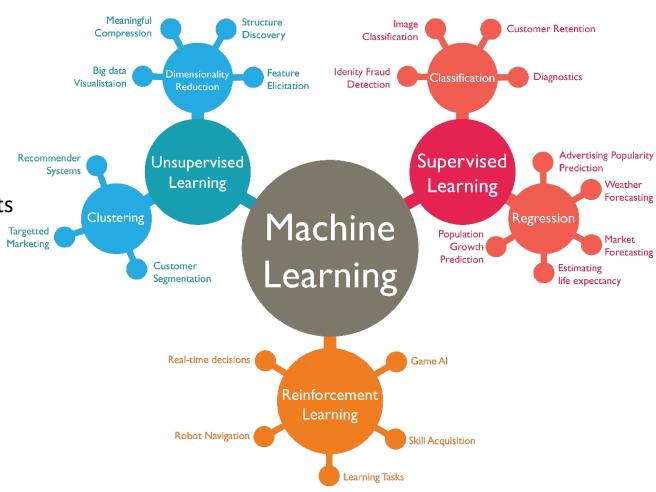






Types of Machine Learning Algorithms

- Supervised (inductive) learning
 - Training data includes desired outputs
 - Classification
 - Regression/Prediction
- Unsupervised learning
 - Training data does not include desired outputs
- Semi-supervised learning
 - Training data includes a few desired outputs
- Reinforcement learning
 - Rewards from sequence of actions

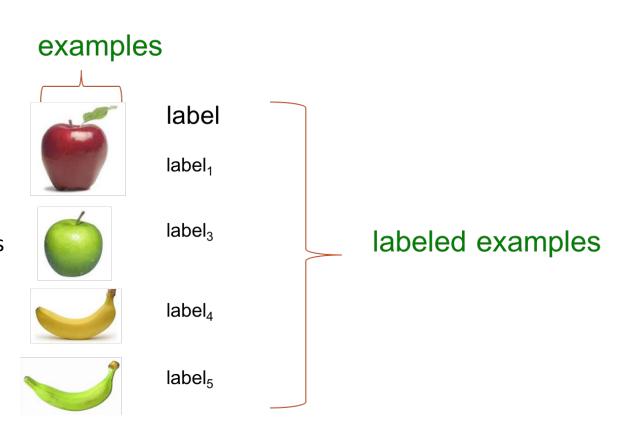






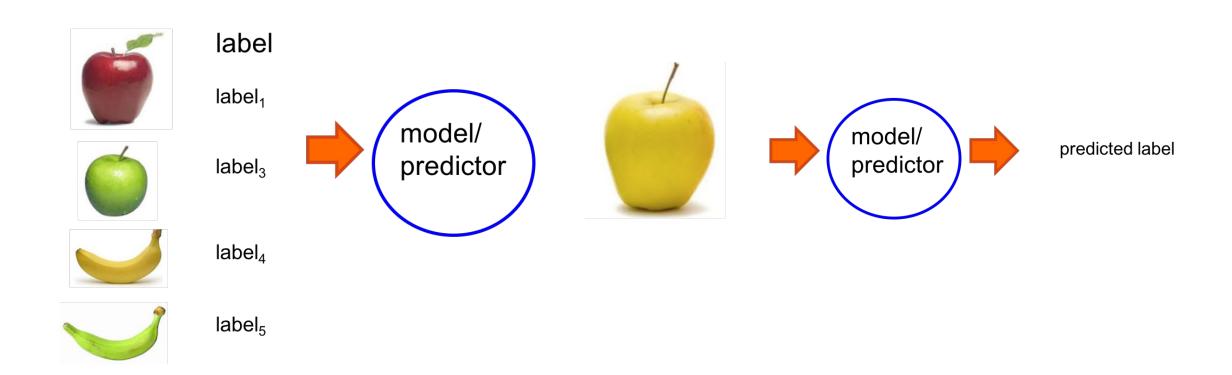
Types of Machine Learning Algorithms

- Supervised (inductive) learning
 - Training data includes desired outputs
 - Classification
 - Regression/Prediction
- Unsupervised learning
 - Training data does not include desired outputs
- Semi-supervised learning
 - Training data includes a few desired outputs
- Reinforcement learning
 - Rewards from sequence of actions







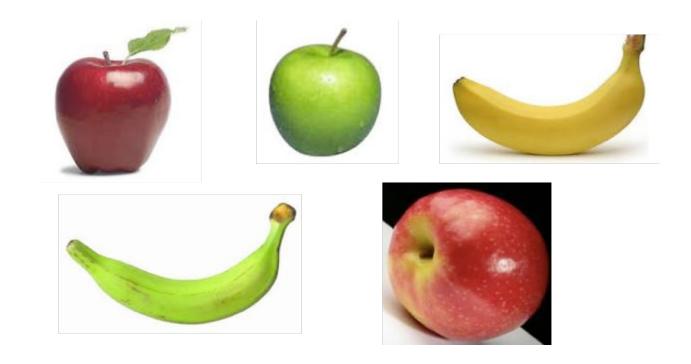






Unsupervised learning: given data, i.e. examples, but no labels

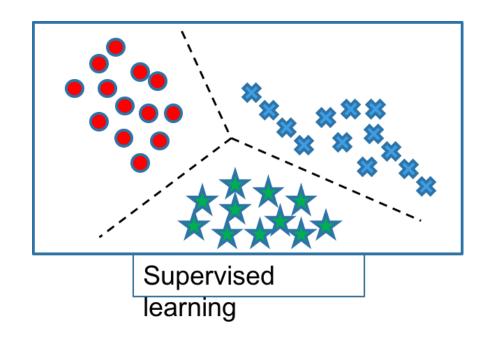
•Clustering: Grouping similar instances

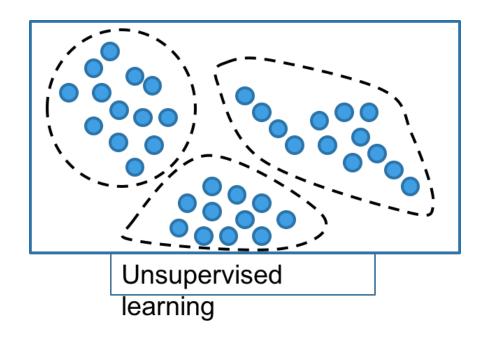






Supervised Versus Un-Supervised learning

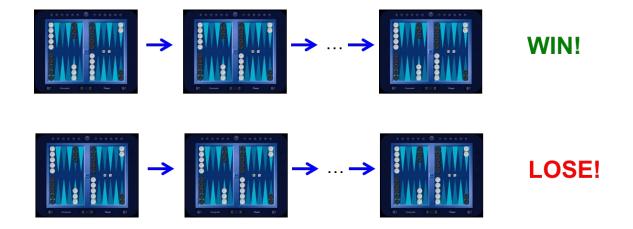








Reinforcement Learning



Given a *sequence* of examples/states and a *reward* after completing that sequence, learn to predict the action to take in for an individual example/state





- Tens of thousands of machine learning algorithms
 - Hundreds new every year
- Every machine learning algorithm has three components:

Representation ----- Evaluation ----- Optimization

Representation

- What is the model design landscape?
- Decision trees
- Sets of rules / Logic programs
- Instances
- Graphical models (Bayes/Markov nets)
- Neural networks
- Support vector machines
- Model ensembles

• ..



Evaluation

- How is the model doing?
- Accuracy
- Precision and recall
- Squared error
- Likelihood
- Posterior probability
- Cost / Utility
- Margin
- Entropy
- K-L divergence

• ...

Optimization

- How can we get better models?
- Combinatorial optimization
 - Greedy search
- Convex optimization
 - Gradient descent
- Nonconvex optimization
 - Stochastic gradient methods
- Constrained optimization
 - Linear programming



Growth of Machine Learning

- Machine learning is preferred approach to
 - Speech recognition, Natural language processing
 - Computer vision
 - Medical outcomes analysis
 - Robot control
 - Web search
 - Finance
 - Social Networks

This trend is accelerating

- Improved machine learning algorithms
- Improved data capture, networking, faster computers
- Software too complex to write by hand
- New sensors / IO devices
- Big Data





Scikit-learn

- Supervised Learning
 - https://scikit-learn.org/stable/supervised learning.html

- Un-Supervised Learning
 - https://scikit-learn.org/stable/unsupervised learning.html
- Implement a model: from sklearn.linear_model import LinearRegression
- Train the model: model.fit()
- Predict: model.predict()
- Visualize the outcome: plt.plot()



Introduction to Machine Learning

 https://github.com/q-tong/CS405-605-Data-Science/blob/main/Fall2023/Lecture/4.Machine%20Learning/Machine_learning/0-Machine_Learning_Overview.ipynb

Introduction to Scikit-Learn: Machine Learning with Python

 https://github.com/q-tong/CS405-605-Data-Science/blob/main/Fall2023/Lecture/4.Machine%20Learning/Machine_learning/1-Machine-Learning-Intro.ipynb

Basic Principles of Machine Learning

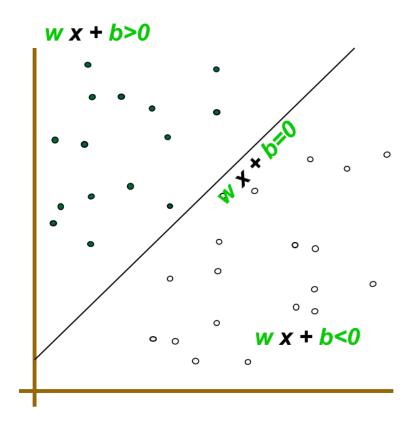
 https://github.com/q-tong/CS405-605-Data-Science/blob/main/Fall2023/Lecture/4.Machine%20Learning/Machine_learning/2-Basic-Principles.ipynb





SVM: Support Vector Machines

- Supervised learning
- Classification (categorical)
- Regression (continuous)







SVM

- Key Concepts
- Hyperplane:

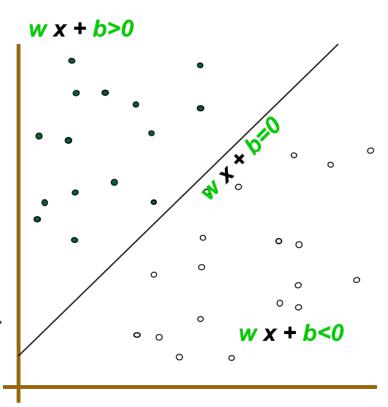
A decision boundary that separates different classes.

Support Vectors:

Data points closest to the hyperplane.

Margin:

Distance between the hyperplane and the support vectors.







SVM

- Key Concepts
- Hyperplane:

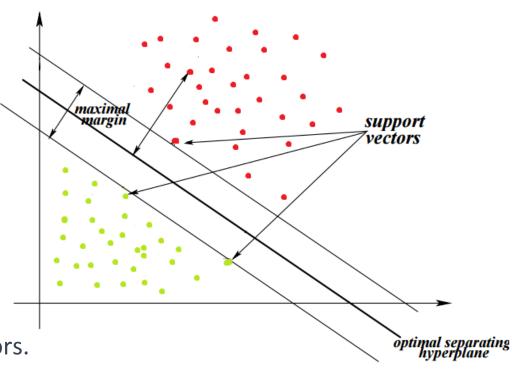
A decision boundary that separates different classes.

Support Vectors:

Data points closest to the hyperplane.

Margin:

Distance between the hyperplane and the support vectors.



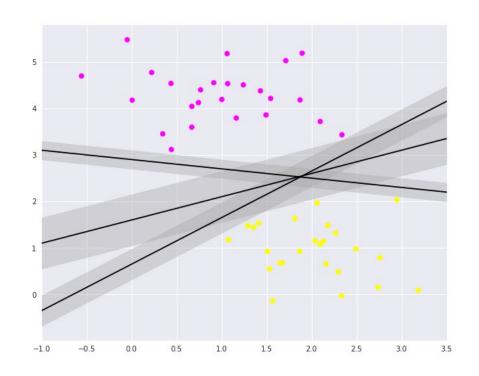
Maximizing the *Margin*





SVM - Maximizing the Margin

What support vector machine does is to not only draw a line,
 but consider a *region* about the line of some given width.







SVM – Scikit-learn

```
from sklearn.svm import SVC # "Support Vector Classifier"
clf = SVC(kernel='linear')
clf.fit(X, y)

SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
    decision_function_shape=None, degree=3, gamma='auto', kernel='linear',
    max_iter=-1, probability=False, random_state=None, shrinking=True,
    tol=0.001, verbose=False)
```

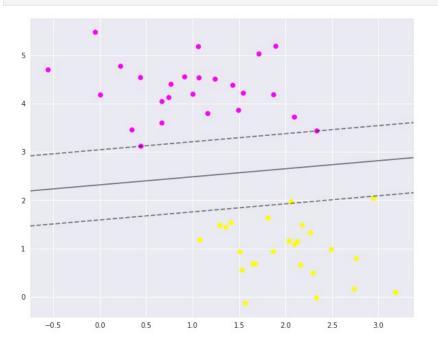




 To better visualize what's happening here, let's create a quick convenience function that will plot SVM decision boundaries for us:

```
def plot svc decision function(clf, ax=None):
    """Plot the decision function for a 2D SVC"""
    if ax is None:
        ax = plt.gca()
    x = np.linspace(plt.xlim()[0], plt.xlim()[1], 30)
    y = np.linspace(plt.ylim()[0], plt.ylim()[1], 30)
    Y, X = np.meshgrid(y, x)
    P = np.zeros like(X)
    for i, xi in enumerate(x):
        for j, yj in enumerate(y):
            P[i, j] = clf.decision function([xi, yj])
    # plot the margins
    ax.contour(X, Y, P, colors='k',
               levels=[-1, 0, 1], alpha=0.5,
               linestyles=['--', '-', '--'])
```

```
plt.figure(figsize=(10,8))
plt.scatter(X[:, 0], X[:, 1], c=y, s=50, cmap='spring')
plot_svc_decision_function(clf);
```



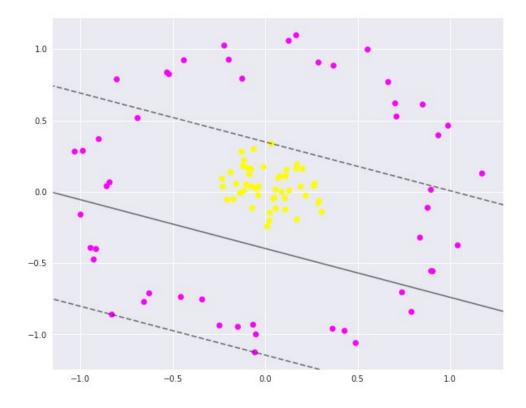




Going further: Kernel Methods

• Where SVM gets incredibly exciting is when it is used in conjunction with kernels.

To motivate the need for kernels, let's look at some data which is not linearly separable:

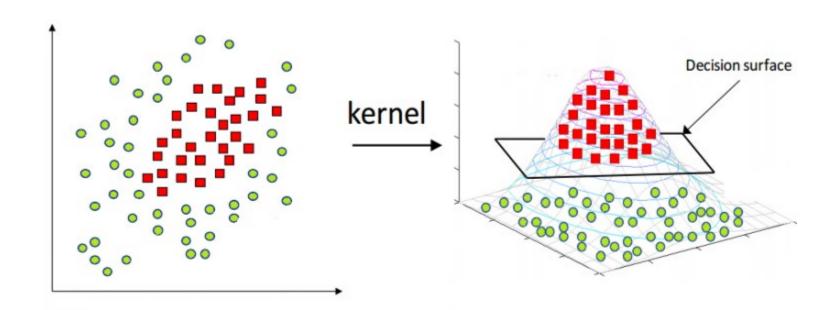




•The *kernel trick* in SVM

- transforms 2-d data into a 3-d space using a *kernel*
- in such a 3-d space a linear hyperplane can be used to separate classes
- Radial basis function (rbf)

$$K(X_i,X_j) = exp(-(X_i^2 + X_j^2))$$





Use rbf:

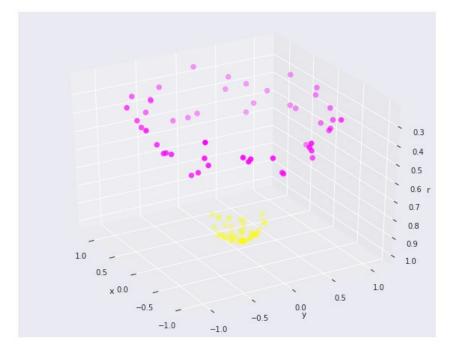
```
r = np.exp(-(X[:, 0] ** 2 + X[:, 1] ** 2))
```

If we plot this along with our data,

```
from mpl_toolkits import mplot3d

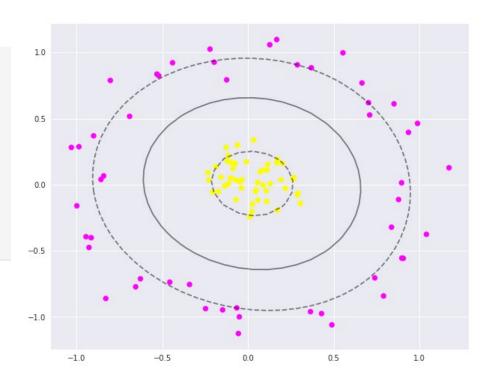
def plot_3D(elev=30, azim=30):
    plt.figure(figsize=(10, 8))
    ax = plt.subplot(projection='3d')
    ax.scatter3D(X[:, 0], X[:, 1], r, c=y, s=50, cmap='spring')
    ax.view_init(elev=elev, azim=azim)
    ax.set_xlabel('x')
    ax.set_ylabel('y')
    ax.set_zlabel('r')

interact(plot_3D, elev=[-150, 150], azip=(-180, 180));
```





• We can see that with this additional dimension, the data becomes trivially linearly separable! This is a relatively simple kernel; SVM has a more sophisticated version of this kernel built-in to the process. This is accomplished by using kernel='rbf', short for radial basis function:





In-Class Exercise: SVM Implementation with the Iris Dataset

Objective: Implement an SVM classifier using the Iris dataset and visualize the decision boundaries. (15 minutes)

Steps:

- Import the necessary libraries.
- Load the Iris dataset.
- Split the dataset into training and testing subsets.
- Implement an SVM classifier and train it on the training subset.
- Evaluate the classifier on the testing subset and print the accuracy.
- Visualize the decision boundaries using appropriate plotting tools.



Example code::

```
# Step 1: Import the necessary libraries
import numpy as np
import matplotlib.pyplot as plt
from sklearn import datasets
from sklearn.svm import SVC
from sklearn.model selection import train test split
from sklearn.metrics import accuracy score
# Step 2: Load the Iris dataset
iris = datasets.load iris()
X = iris.data[:, :2] # taking only the first two features for easy visualization
y = iris.target
# Step 3: Split the dataset into training and testing subsets
X train, X test, y train, y test = train test split(X, y, test size=0.3, random state=42)
# Step 4: Implement an SVM classifier and train it
clf = SVC(kernel='linear')
clf.fit(X train, y train)
         SVC
SVC(kernel='linear')
```



```
# Step 5: Evaluate the classifier
y_pred = clf.predict(X_test)
print(f"Accuracy: {accuracy_score(y_test, y_pred) * 100:.2f}%")
Accuracy: 80.00%
# Step 6: Visualize the decision boundaries
plt.figure(figsize=(10, 6))
plt.scatter(X[:, 0], X[:, 1], c=y, edgecolors='k', cmap=plt.cm.Paired)
ax = plt.gca()
xlim = ax.get xlim()
ylim = ax.get ylim()
# create a grid to evaluate model
xx = np.linspace(xlim[0], xlim[1], 50)
yy = np.linspace(ylim[0], ylim[1], 50)
YY, XX = np.meshgrid(yy, xx)
xy = np.vstack([XX.ravel(), YY.ravel()]).T
Z = clf.decision function(xy)
# For multiclass SVM, get the class with the maximum decision function value for each point
Z = np.argmax(Z, axis=1).reshape(XX.shape)
# plot decision boundary
contour = ax.contourf(XX, YY, Z, alpha=0.8, cmap=plt.cm.Paired)
# plot support vectors
ax.scatter(clf.support_vectors_[:, 0], clf.support_vectors_[:, 1], s=100, facecolors='none', edgecolors='k')
plt.show()
```



