Machine Learning (CE 40717)

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1. Introduction to Classification
2. Discriminant Functions
3. Linear Classifiers
4. Perceptron
5. Cost Functions
6. Cross Validation
7. Multi-Category Classification
8. References

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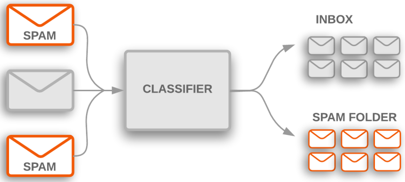
Definition

- Given: Training Set
  - A dataset D with N labeled instances $D = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^{N}$
  - $y^{(i)} \in \{1, \dots, K\}$
- Goal: Given an input x, assign it to one of K classes.
- Real-World Examples:
  - Email Spam Detection
  - Medical Diagnosis
  - Churn Prediction



Real-World Example of Classification

- **Pima Indians Diabetes Dataset:**
  - **Problem**: Predict whether a patient has diabetes based on medical diagnostics.
  - **Context**: Early detection of diabetes is critical for treatment and management.

	Number of times pregnant	Glucose	Blood Pressure	Skin Thickness	Insulin	Diabetes pedigree function	Age	BMI	Label
Patient 1	6	148	72	35	0	0.627	50	33.6	Positive
Patient 2	1	85	66	29	0	0.351	31	26.6	Negative
Patient 3	0	137	40	35	168	2.288	33	43.1	Positive
Patient 4	1	89	66	23	94	0.167	21	28.1	Negative
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

Classification vs. Regression

Aspect	Linear Regression	Linear Classification
Output Type	Continuous values (real numbers).	Binary or Multi-class labels (e.g., -1/+1, A/B/C)
Use Cases	Predicting house prices, stock market trends.	Email spam detection, Credit Scoring, Churn Prediction

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Discriminant Functions in Machine Learning

- **Definition**
  - A function that assigns a score to an input vector x, to classify it into different classes.
  - It maps the input $\mathbf{x}$ to a real number $g(\mathbf{x})$, which represents the degree of confidence in assigning $\mathbf{x}$ to a particular class.

Discriminant Functions in Machine Learning

- **How it works**
  - **Binary Classification**: Two functions $g_1(\mathbf{x})$ and $g_2(\mathbf{x})$ for classes C_1 and C_2, respectively. The class is predicted by comparing these two functions:

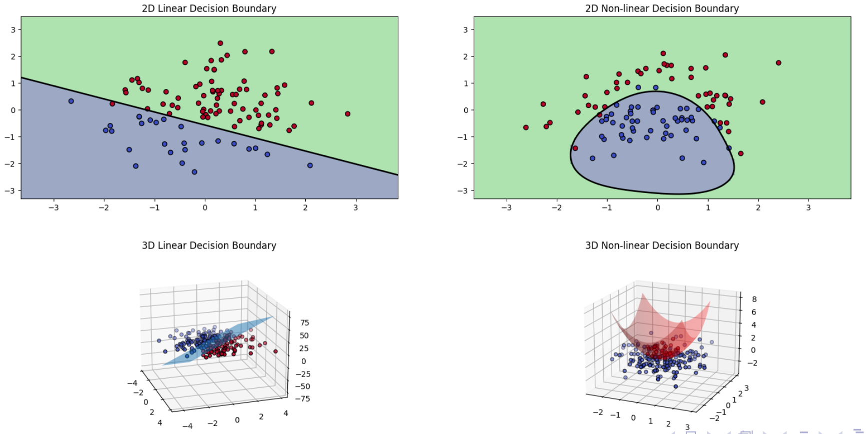
$$\hat{y} = \begin{cases} C_1 & \text{if } g_1(\mathbf{x}) > g_2(\mathbf{x}) \\ C_2 & \text{otherwise} \end{cases}$$

  - **General Case**: For k-class problems, we compute $g_i(\mathbf{x})$ for every class i, and assign x to class with highest score:

$$\hat{y} = \arg\max_i g_i(\mathbf{x})$$

Decision Boundary

- **Definition**: A dividing hyperplane that separates different classes in a feature space, also known as "Decision Surface".



Discriminant Functions: Two-Category

- **Function**: For two-category problem, we can only find a function $g : \mathbb{R}^d \to \mathbb{R}$
  - $g_1(\mathbf{x}) = g(\mathbf{x})$,
  - $g_2(\mathbf{x}) = -g(\mathbf{x})$
- **Decision Boundary**: $g(\mathbf{x}) = 0$
- At first, we start by explaining two-category classification for simplicity, and then extend the concept to multi-category classification for more complex problems.

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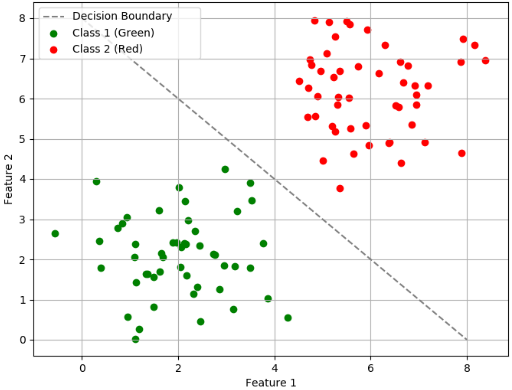
Linear Classifiers

- **Definition**: In case of linear classifiers, decision boundaries are linear in d ($\mathbf{x} \in \mathbb{R}^d$), or linear in some given set of functions of x.
- **Linearly separable data**: Data points that can be exactly separated by a linear decision boundary.
- **Why are they popular?**
  - Simplicity, Efficiency, Effectiveness.

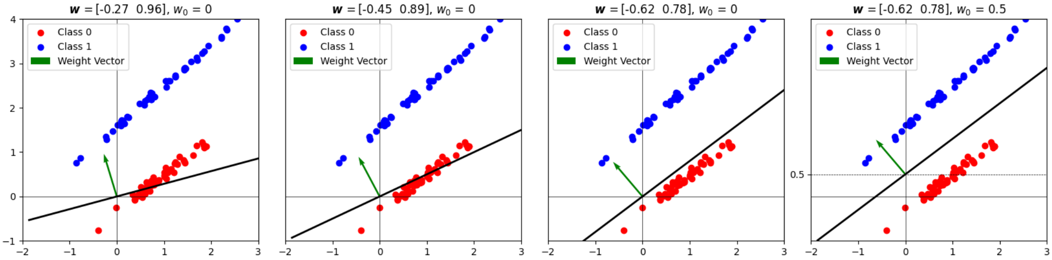
Two Category Classification

- $g(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + w_0 = w_d \cdot x_d + \ldots + w_1 \cdot x_1 + w_0$
  - $\mathbf{x} = [x_1 \ \ldots \ x_d]$
  - $\mathbf{w} = [w_1 \ \ldots \ w_d]$
  - w_0: bias
- $\begin{cases} C_1 & \text{if } \mathbf{w}^T\mathbf{x} + w_0 \geq 0 \\ C_2 & \text{otherwise} \end{cases}$
- **Decision Surface**: $\mathbf{w}^T\mathbf{x} + w_0$



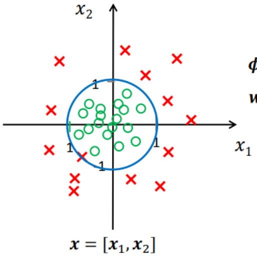
Two Category Classification Cont.

- Decision Boundary is a $(d-1)$-dimensional hyperplane H in the d-dimensional feature space. Some properties of H are:
  - Orientation of H is determined by the normal vector $[\frac{w_1}{\|w\|}, \ldots, \frac{w_d}{\|w\|}]$.
  - w_0 determines the location of the surface.



Non-linear decision boundary

- **Non-linear Decision Boundaries**
  - **Feature Transformation**: Non-linearity is introduced by transforming features into a higher-dimensional space.
  - **Linear in Transformed Space**: The decision boundary becomes linear in the new space, but non-linear in the original space.



$-1 + x_1^2 + x_2^2 = 0$

$\boldsymbol{\phi}(\boldsymbol{x}) = [1, x_1, x_2, x_1^2, x_2^2, x_1 x_2]$

$\boldsymbol{w} = [w_0, w_1, \ldots, w_m] = [-1, 0, 0, 1, 1, 0]$

if $\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}) \geq 0$ then $y = 1$
else $y = -1$

Figure adapted from slides of M. Soleymani, Machine Learning course, Sharif University of Technology.

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What Is Perceptron?

- **Perceptron Unit**:
  - **Basic Building Block**: A perceptron is the simplest type of artificial neuron used in machine learning.
  - **Linear Classifier**: It maps input features to an output by applying a linear combination and a threshold.
  - **Binary Decision**: Outputs 1 if the weighted sum of inputs exceeds the threshold, otherwise 0.
  - **Components**: Inputs, weights, bias, and an activation function (often a step or a sigmoid function).

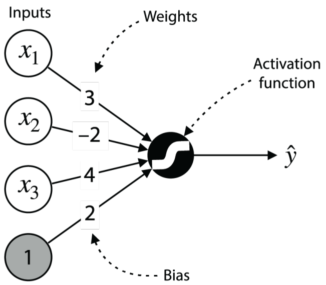
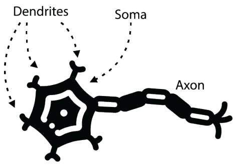


Figure adapted from Grokking Machine Learning, L. G. Serrano.

Inspired by Biology

- **Biological Motivation Behind Perceptron:**
  - **Inspired by Neurons**: Perceptron mimics the basic function of biological neurons in the brain.
    - Input and Output, Activation Function.



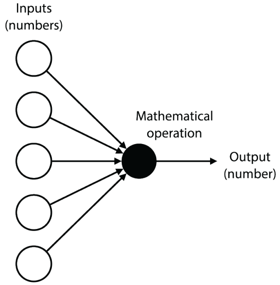


Figure adapted from Grokking Machine Learning, L. G. Serrano.

Single Neuron

- **Single Neuron as a Linear Decision Boundary**
  - **Mathematical Form**: The output of a single neuron is computed as:
    $$y = f(\mathbf{w}^T\mathbf{x} + w_0)$$
    where:
    - $\mathbf{x}$ is the input vector.
    - $\mathbf{w}$ is the weight vector.
    - w_0 is the bias term.
    - f is an activation function (e.g., step function).
  - **Linear Separation**: A neuron defines a linear decision boundary:
    $\mathbf{w}^T\mathbf{x} + w_0 = \textit{threshold}$ (0 for step, 0.5 for sigmoid)
  - **Decision Rule**: C_1 if $\mathbf{w}^T\mathbf{x} + w_0 \geq \textit{threshold}$, otherwise C_2.

$$\text{Class} = f(\mathbf{w}^T\mathbf{x} + w_0)$$

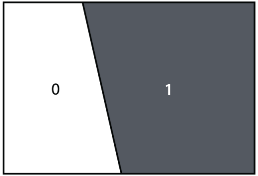
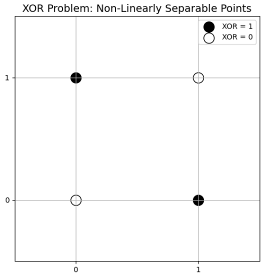


Figure adapted from Grokking Machine Learning, L. G. Serrano.

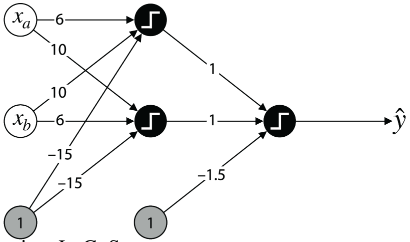
Limitations of a Single Perceptron

- **What a Single Perceptron Can and Can't Do:**
  - **Performs Linear Separations:** A perceptron can handle linearly separable problems such as:
    - AND operation
    - OR operation
  - **Fails on Non-Linear Problems:** A single perceptron fails to solve non-linear problems like XOR, as the data points cannot be separated by a straight line.



Towards Complex Decision Boundaries

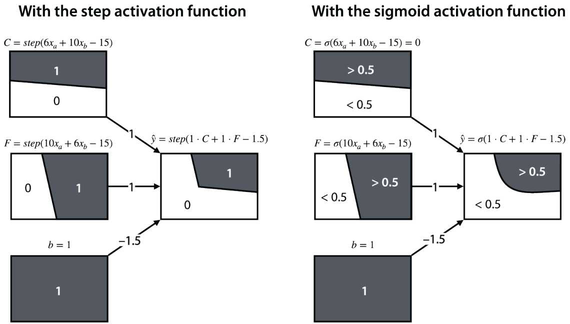
- **Multi-Layer Perceptron (MLP):**
  - **Adding Layers for More Complexity**: An MLP consists of multiple layers of neurons that allow us to model more complex functions than a single neuron.
    - Each layer introduces new decision boundaries, making it possible to separate non-linear data.
  - **Two-Layer Example:**
    - Input Layer → Hidden Layer → Output Layer
    - Hidden layer introduces non-linear transformations that enable complex decision regions.



Figures adapted from Grokking Machine Learning, L. G. Serrano.

Refining the Decision Boundary

- **New Neurons for Better Separation**: By adding more neurons to a layer, we can further refine the decision boundary to better separate complex data.
- Each additional neuron introduces new features that help the model make more accurate decisions.



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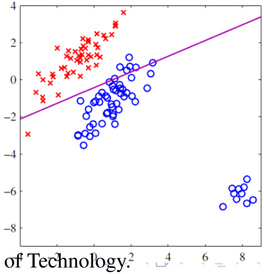
Cost Functions

- **Understanding the Goal**
  - In the perceptron, we use $\mathbf{w}^T\mathbf{x}$ to make predictions.
  - Goal is to find the optimal $\mathbf{w}$ so that the predicted labels match the true labels as much as possible.
  - To achieve this, we define a cost function, which measures the **difference** between **predicted** and **actual** labels.
  - Finding discriminant functions $(\mathbf{w}^T, w_0)$ is framed as minimizing a cost function.
    - Based on training set $D = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^{N}$, a cost function $J(\mathbf{w})$ is defined.
    - Problem converts to finding optimal $\hat{g}(\mathbf{x}) = g(\mathbf{x}; \hat{\mathbf{w}})$ where

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w}} J(\mathbf{w})$$

Sum of Squared Error Cost Function

- **Sum of Squared Error (SSE) Cost Function**
  - **Formula**: $J(\mathbf{w}) = \sum_{i=1}^{n} (y^{(i)} - \hat{y}^{(i)})^2, \quad \hat{y}^{(i)} = \mathbf{w}^T \mathbf{x}^{(i)} + w_0$
  - SSE minimizes the magnitude of the error, which is ideal for regression but irrelevant for classification.
  - If the model predicts close to the true class but not exactly 0 or 1, SSE still shows positive error, even for correct predictions.
- SSE is also prone to overfitting noisy data, as small variations can cause significant changes in the cost.



Figures adapted from slides of M. Soleymani, Machine Learning course, Sharif University of Technology.

An Alternative for SSE Cost Function

- **Number of Misclassifications**
  - **Definition**: Measures how many samples are misclassified by the model.
  - **Formula**:

$$J(\mathbf{w}) = \sum_{i=1}^{n} (y^{(i)} - \text{sign}(\hat{y}^{(i)}))^2, \quad \hat{y}^{(i)} = \mathbf{w}^T \mathbf{x}^{(i)} + w_0, \quad y^{(i)} \in \{-1, +1\}$$

  - **Limitations**:
    - **Piecewise Constant**: The cost function is non-differentiable, so optimization techniques (like gradient descent) cannot be directly applied.

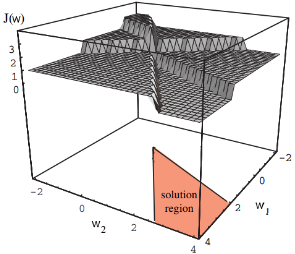
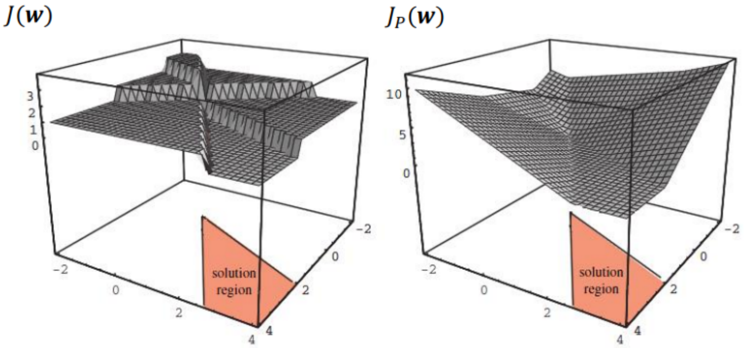


Figure adapted from Machine Learning and Pattern Recognition, Bishop

Perceptron Algorithm

- **The Perceptron Algorithm**
  - **Purpose**: A simple algorithm for binary classification, separating two classes with a linear boundary.



Figures adapted from Machine Learning and Pattern Recognition, Bishop

Perceptron Criterion

- **Cost Function**: The perceptron criterion focuses on misclassified points:

$$J_p(\mathbf{w}) = -\sum_{i \in M} y^{(i)}\, \mathbf{w}^T \mathbf{x}^{(i)}, \quad y^{(i)} \in \{-1, +1\}$$

  where M is the set of misclassified points.

- **Goal**: Minimize the loss by correctly classifying all points.

Batch Perceptron

- **Batch Perceptron**: Updates the weight vector using all misclassified points in each iteration.

- **Gradient Descent**: Adjusting weights in the direction that reduces the loss:

$$\mathbf{w} \leftarrow \mathbf{w} - \eta \nabla_{\mathbf{w}} J_p(\mathbf{w})$$

$$\nabla_{\mathbf{w}} J_p(\mathbf{w}) = -\sum_{i \in M} y_i \mathbf{x}_i$$

  - Batch Perceptron converges in finite number of steps for linearly separable data.

Single-sample Perceptron

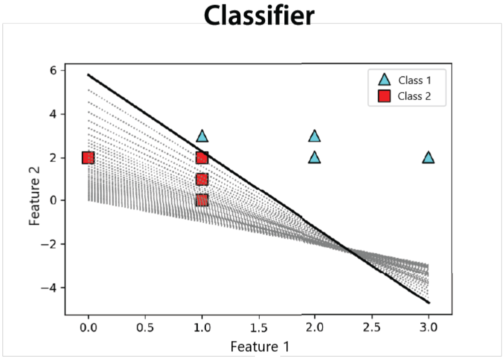
- **Single Sample Perceptron**: Updates the weight vector after each individual point.
- **Stochastic Gradient Descent (SGD) Update Rule:**
  - Using only one misclassified sample at a time:

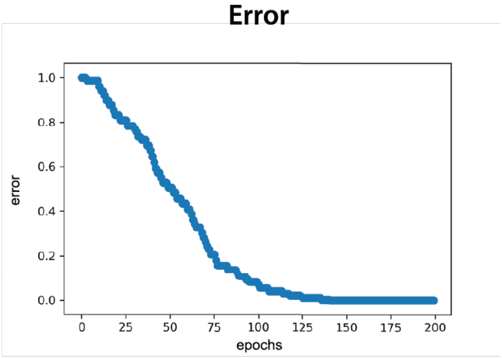
$$\mathbf{w} \leftarrow \mathbf{w} + \eta y_i \mathbf{x}_i$$

  - Lower computational cost per iteration, faster convergence.
  - If training data are linearly separable, the single-sample perceptron is also guaranteed to find a solution in a finite number of steps.

Example

- Perceptron changes **w** in a direction that corrects error.





Figures adapted from Grokking Machine Learning, L. G. Serrano.

Convergence of Perceptron

- **Non-Linearly Separable Data**: When no linear decision boundary can perfectly separate the classes, the Perceptron fails to converge.
  - If data is not linearly separable, there will always be some points that the model fails to classify.
  - As a result, the algorithm keeps adjusting the weights to fix the misclassified points, causing it to never converge.
  - For the data that are not linearly separable due to noise, **Pocket Algorithm** keeps in its pocket the best **w** encountered up to now.

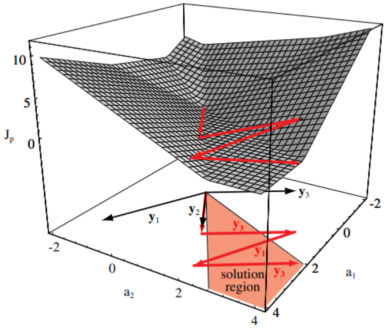


Figure adapted from Machine Learning and Pattern Recognition, Bishop

Pocket Algorithm

Algorithm 1 Pocket Algorithm

```
Initialize w
for t = 1 to T do
    i ← t mod N
    if x^(i) is misclassified then
        w^new = w + η x^(i) y^(i)
        if E_train(w^new) < E_train(w) then
            w = w^new
        end if
    end if
end for
```

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Model Selection via Cross Validation

- **Cross-Validation**
  - **Purpose**: Technique for evaluating how well a model generalizes to unseen data.
  - **How It Works**: Split data into k folds; train on $k-1$ folds and validate on the remaining fold.
  - **Repeat Process**: Repeat k times, rotating the test fold each time. Average of all scores is the final score of the model.
  - Cross-validation reduces overfitting and provides a more reliable estimation of model performance.

K-Fold Cross Validation

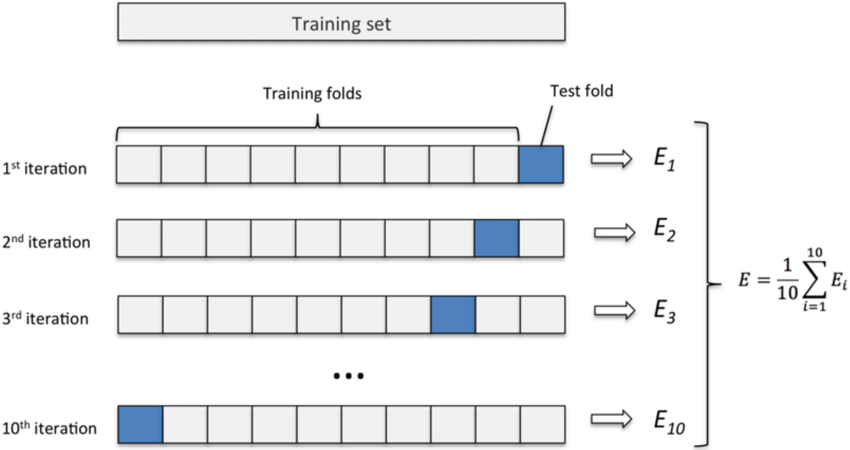
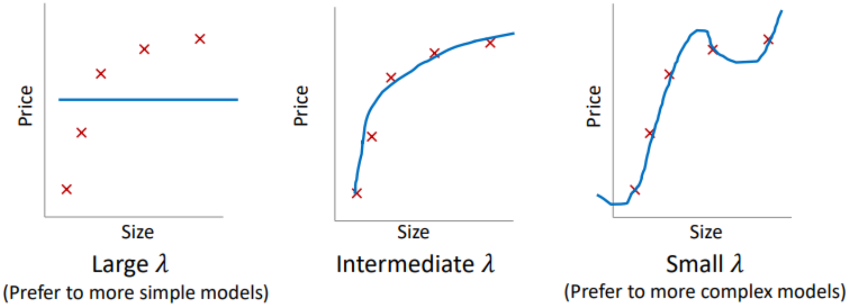


Figure adapted from Introduction to Support Vector Machines and Kernel Methods, J.M. Ashfaque.

Leave-One-Out Cross-Validation (LOOCV)

- **Leave-One-Out Cross-Validation (LOOCV)**
  - **How It Works**: Uses a single data point as the validation set ($k = 1$) and the rest as the training set. Repeat for all data points.
  - **Properties:**
    - **No Data Wastage**: Every data point is used for both training and validation.
    - **High Variance, Low Bias**.
    - **Computationally Expensive**: Requires training the model N times for N data points, making it slow for large datasets.
    - **Best for small datasets**.

Cross-Validation for Choosing Regularization Term



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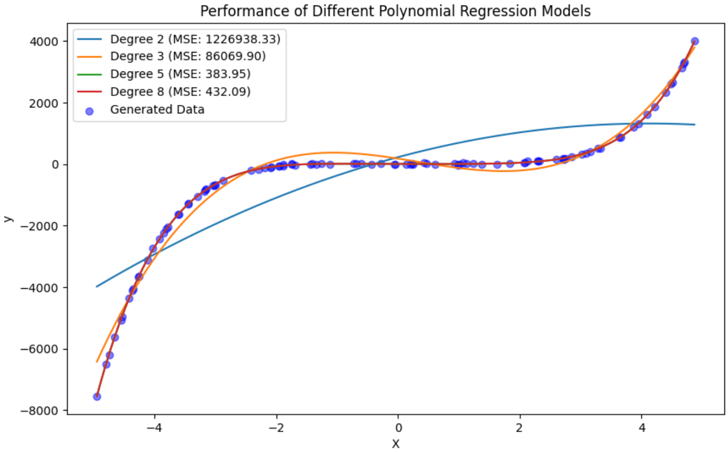
Cross-Validation for Choosing Model Complexity



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Multi-Category Classification

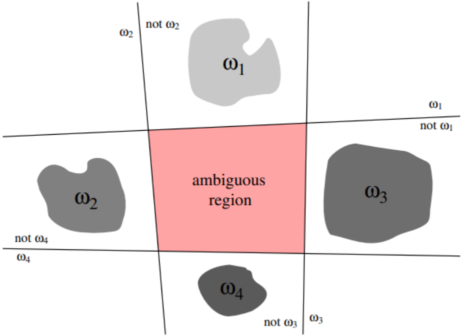
- **Solutions to multi-category classification problem**:
  - Extend the learning algorithm to support multi-class.
    - First, a function g_i for every class C_i is found.
    - Second, $\mathbf{x}$ is assigned to C_i if $g_i(\mathbf{x}) > g_j(\mathbf{x}) \quad \forall i \neq j$

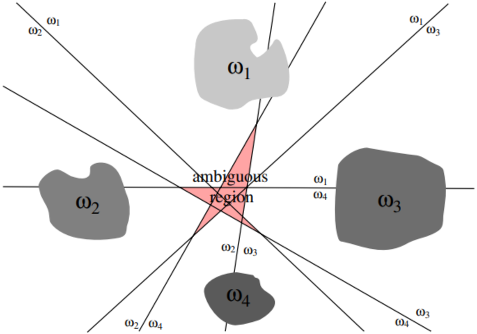
$$\hat{y} = \underset{i=1,\ldots,c}{\operatorname{argmax}}\, g_i(\mathbf{x})$$

  - Convert to a set of two-categorical problems.
    - Methods like **One-vs-Rest** or **One-vs-One**, where each classifier distinguishes between either **one class and the rest**, or **between pairs of classes**.

Multi-Category Classification: Ambiguity

- One-vs-One and One-vs-Rest conversion can lead to regions in which the classification is **undefined**.





Figures adapted from Machine Learning and Pattern Recognition, Bishop

Multi-Category Classification: Linear Machines

- **Linear Machines**: Alternative to One-vs-Rest and One-vs-One methods; Each class is represented by its own discriminant function.

- **Decision Rule:**

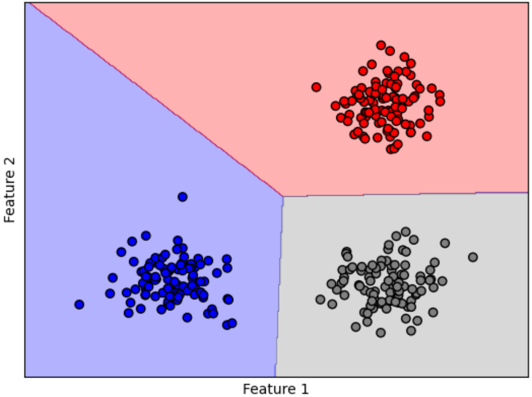
$$\hat{y} = \underset{i=1,\ldots,c}{\operatorname{argmax}}\, g_i(\mathbf{x})$$

The predicted class is the one with the highest discriminant function value.

- **Decision Boundary**: $g_i(\mathbf{x}) = g_j(\mathbf{x})$

$$(\mathbf{w}_i - \mathbf{w}_j)^T \mathbf{x} + (w_{0i} - w_{0j}) = 0$$

Linear Machines Cont.



- The decision regions of this discriminant are **convex** and **singly connected**. Any point on the line between two points within the same region can be expressed as $\mathbf{x} = \lambda \mathbf{x}_A + (1 - \lambda)\mathbf{x}_B$ where $\mathbf{x}_A, \mathbf{x}_B \in C_k$.

Multi-Class Perceptron Algorithm

- **Weight Vectors**:
  - Maintain a weight matrix $W \in \mathbb{R}^{m \times K}$, where m is the number of features and K is the number of classes.
  - Each column w_k of the matrix corresponds to the weight vector for class k.

$$\hat{y} = \underset{i=1,\ldots,c}{\operatorname{argmax}}\, \mathbf{w}_i^T \mathbf{x}$$

$$J_p(\mathbf{W}) = -\sum_{i \in M} (\mathbf{w}_{y^{(i)}} - \mathbf{w}_{\hat{y}^{(i)}})^T \mathbf{x}^{(i)}$$

where M is the set of misclassified points.

Multi-Class Perceptron Algorithm

Algorithm 2 Multi-class perceptron

1: **Initialize** $\mathbf{W} = [\mathbf{w}_1, \ldots, \mathbf{w}_c]$, $k \leftarrow 0$
2: **while** A pattern is misclassified **do**
3: $\quad k \leftarrow k + 1 \bmod N$
4: $\quad$ **if** $\mathbf{x}^{(i)}$ is misclassified **then**
5: $\quad\quad \mathbf{w}_{\hat{y}^{(i)}} = \mathbf{w}_{\hat{y}^{(i)}} - \eta \mathbf{x}^{(i)}$
6: $\quad\quad \mathbf{w}_{y^{(i)}} = \mathbf{w}_{y^{(i)}} + \eta \mathbf{x}^{(i)}$
7: $\quad$ **end if**
8: **end while**

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Contributions

- **This slide has been prepared thanks to:**
  - Erfan Jafari

[1] C. M. Bishop, *Pattern Recognition and Machine Learning*.

[2] R. O. Duda, P. E. Hart, and D. G. Stork, *Pattern Classification*.
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