Machine Learning (CE 40717)

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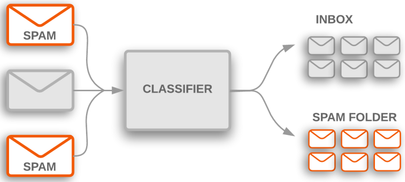
Definition

- 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

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:

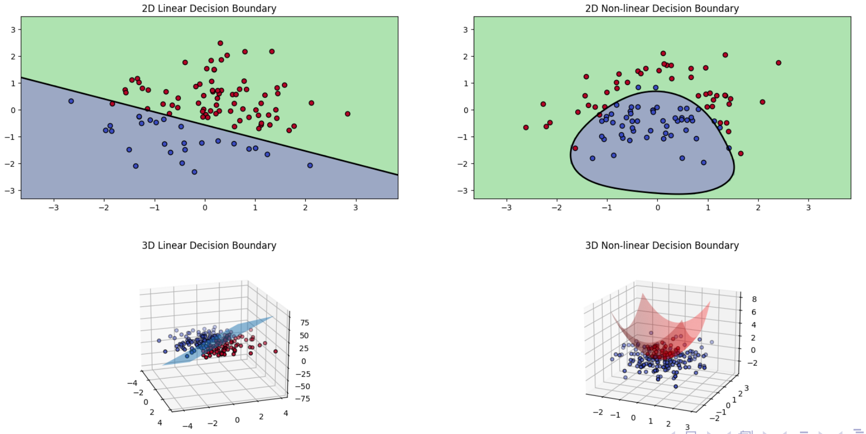
$$\hat{y} = \begin{cases} C_1 & \text{if } g_1(\mathbf{x}) > g_2(\mathbf{x}) \\ C_2 & \text{otherwise} \end{cases}$$

  - **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

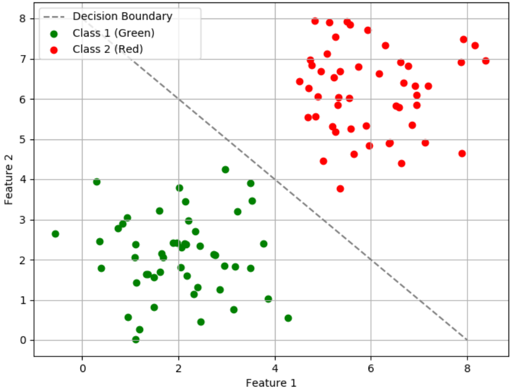
- **Function**: For two-category problem, we can only find a function $g : \mathbb{R}^d \to \mathbb{R}$
  - $g_1(\mathbf{x}) = g(\mathbf{x})$,
  - $g_2(\mathbf{x}) = -g(\mathbf{x})$
- **Decision Boundary**: $g(\mathbf{x}) = 0$
- At first, we start by explaining two-category classification for simplicity,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

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.

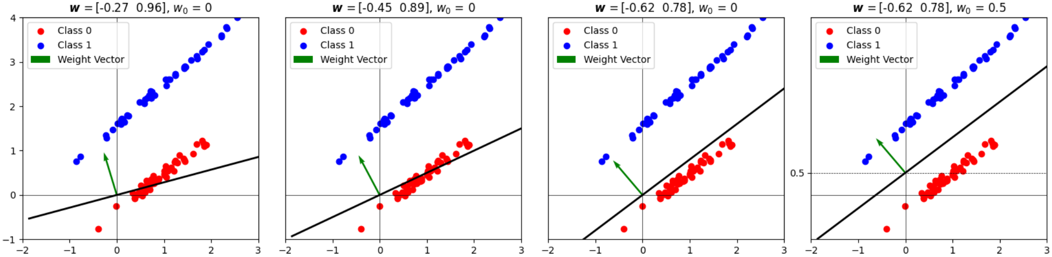
Two Category Classification

- $g(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + w_0 = w_d \cdot x_d + \ldots + w_1 \cdot x_1 + w_0$
  - $\mathbf{x} = [x_1 \ldots x_d]$
  - $\mathbf{w} = [w_1 \ldots w_d]$
  - 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**: $\mathbf{w}^T\mathbf{x} + w_0$



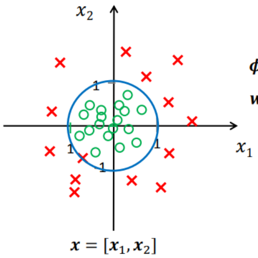
Two Category Classification Cont.

- 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.



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

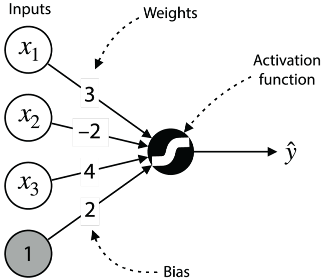
$\phi(x) = [1, x_1, x_2, x_1^2, x_2^2, x_1 x_2]$

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

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

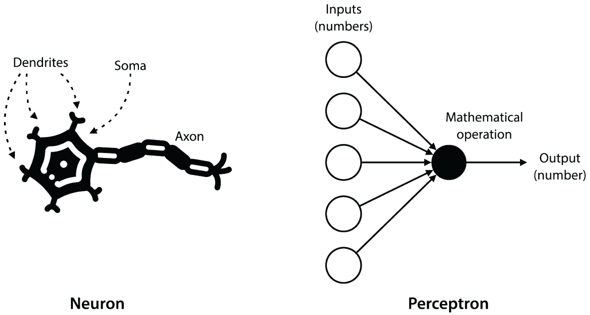
What Is Perceptron?

- **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).



Inspired by Biology

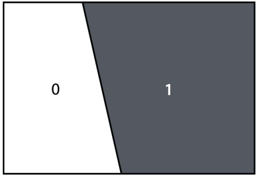
- **Biological Motivation Behind Perceptron:**
  - **Inspired by Neurons**: Perceptron mimics the basic function of biological neurons in the brain.
    - Input and Output, Activation Function.



Single Neuron

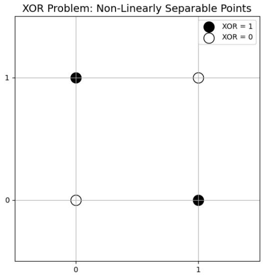
- **Single Neuron as a Linear Decision Boundary**
  - **Mathematical Form**: The output of a single neuron is computed as:
  $$y = f(\mathbf{w}^T\mathbf{x} + w_0)$$
  where:
    - $\mathbf{x}$ is the input vector.
    - $\mathbf{w}$ is the weight vector.
    - w_0 is the bias term.
    - f is an activation 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.

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



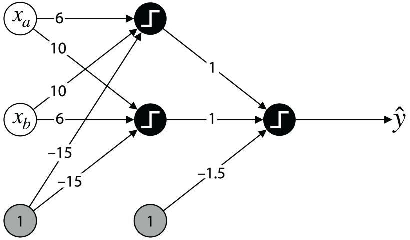
Limitations of a Single Perceptron

- **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.



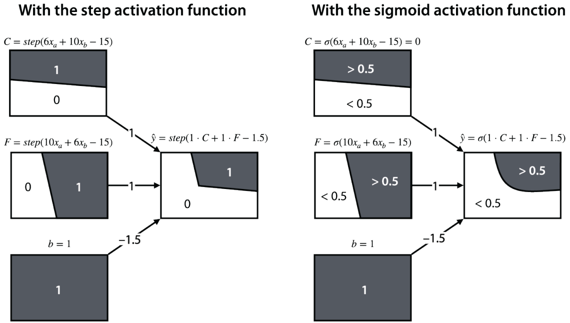
Towards Complex Decision Boundaries

- **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.



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.



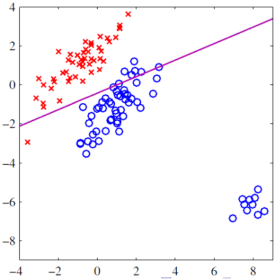
Cost Functions

- **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 C_1 or C_2, 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.

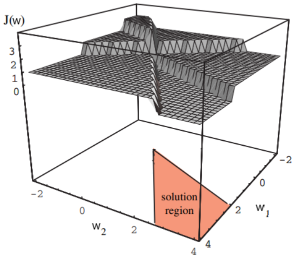


An Alternative for SSE Cost Function

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

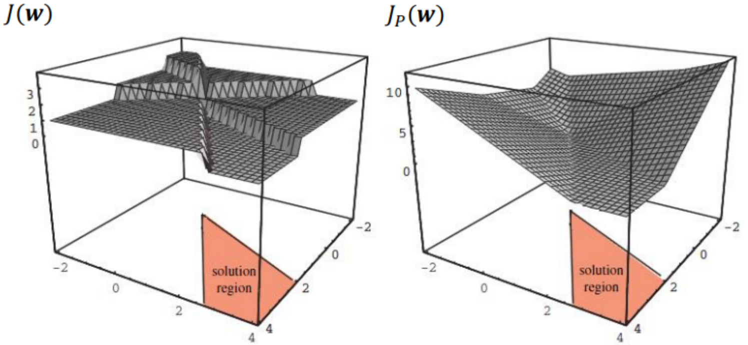
$$J(\mathbf{w}) = \sum_{i=1}^{n} (y^{(i)} - \text{step}(\hat{y}^{(i)}))^2, \quad \hat{y}^{(i)} = \mathbf{w}^T \mathbf{x}^{(i)} + w_0$$

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



Perceptron Algorithm

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



Perceptron Criterion

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

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

  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

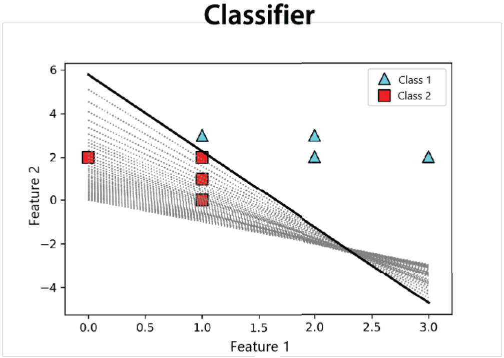
- **Single Sample Perceptron**: Updates the weight vector after each individual point.
- **Stochastic Gradient Descent (SGD) Update Rule:**
  - Using only one misclassified sample at a time:

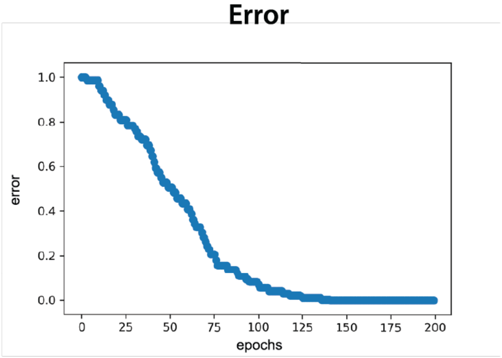
$$\mathbf{w} \leftarrow \mathbf{w} + \eta y_i \mathbf{x}_i$$

  - 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

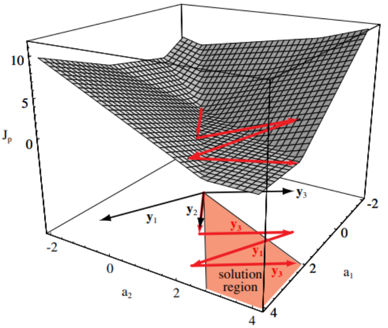
- Perceptron changes **w** in a direction that corrects error.





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.



Pocket Algorithm

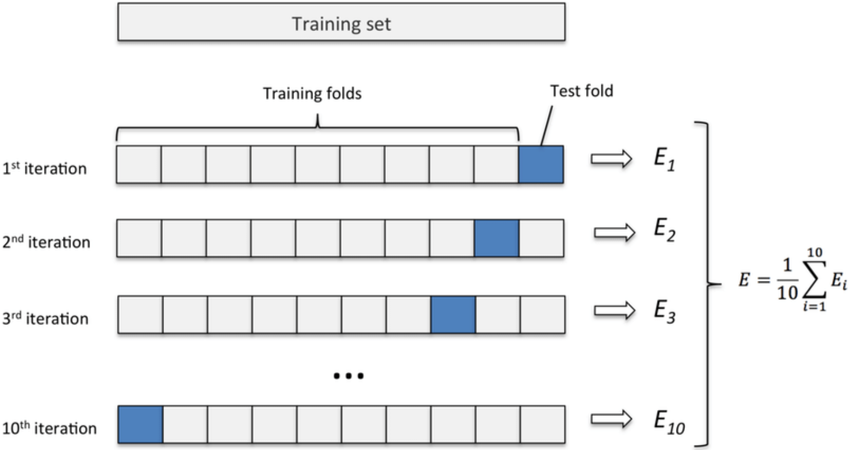
Algorithm 1 Pocket Algorithm

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

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.

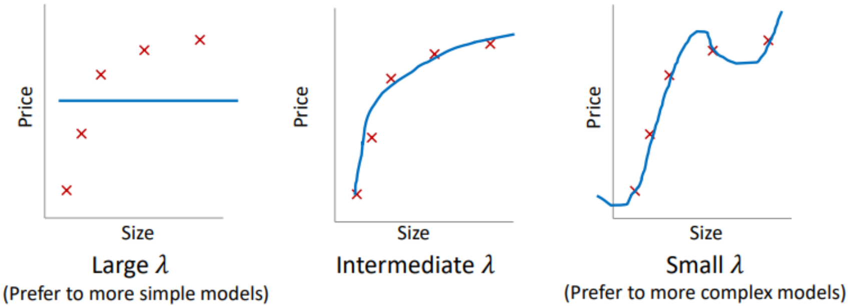
K-Fold Cross Validation



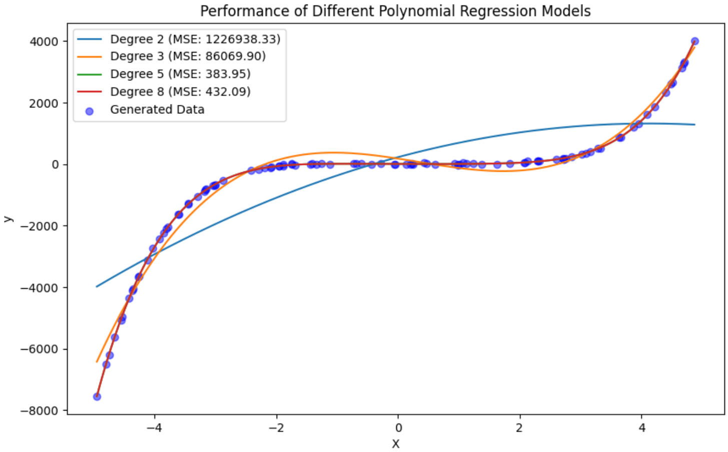
Leave-One-Out Cross-Validation (LOOCV)

- **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



Cross-Validation for Choosing Model Complexity



Multi-Category Classification

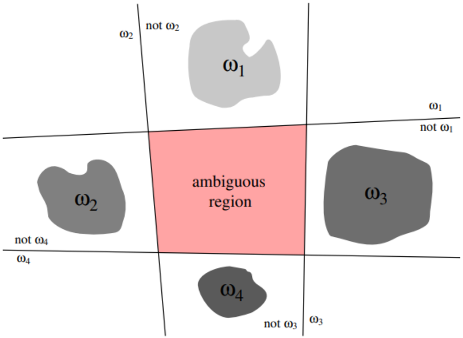
- **Solutions to multi-category classification problem**:
  - Extend the learning algorithm to support multi-class.
    - First, a function g_i for every class C_i is found.
    - Second, $\mathbf{x}$ is assigned to C_i if $g_i(\mathbf{x}) > g_j(\mathbf{x}) \quad \forall i \neq j$

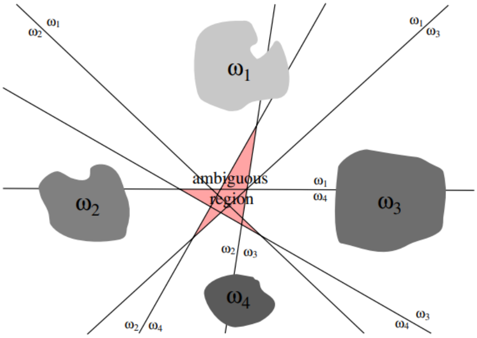
$$\hat{y} = \underset{i=1,\ldots,c}{\operatorname{argmax}}\, g_i(\mathbf{x})$$

  - 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**.





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:**

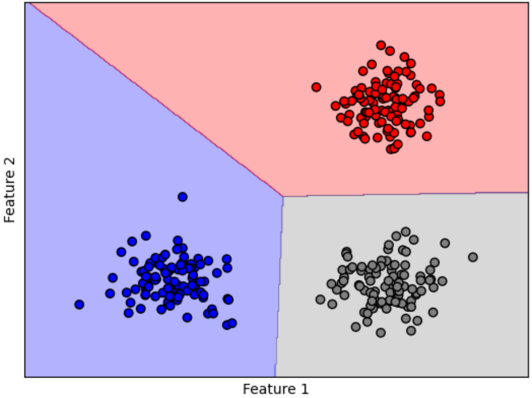
$$\hat{y} = \underset{i=1,\ldots,c}{\operatorname{argmax}}\, g_i(\mathbf{x})$$

  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: $\quad\quad \mathbf{w}_{\hat{y}^{(i)}} = \mathbf{w}_{\hat{y}^{(i)}} - \mathbf{x}^{(i)}$
6: $\quad\quad \mathbf{w}_{y^{(i)}} = \mathbf{w}_{y^{(i)}} + \mathbf{x}^{(i)}$
7: $\quad$ **end if**
8: **end while**

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