Machine Learning (Lab support)
Multi-class classification

Abdelkrime Aries   Leila Hamdad   Karima Benatchba

Laboratoire de la Communication dans les Systèmes Informatiques (LCSI)

Laboratoire des Méthodes de Conception des Systèmes (LMCS)

École nationale Supérieure d'Informatique (ESI, ex. INI), Alger, Algérie

Academic year: 2023/2024

Machine Learning

Multi-class classification: Introduction

- We have already seen ...
  - how to estimate the probability of a class
  - using logistic regression
  - in case of binary classification (belongs to a class or not)
- But ...
  - how to estimate them in case of multiple classes?
  - how to affect a sample into many classes at once?

Machine Learning

Multi-class classification: Plan

1. **Classification**
   - Binary classification
   - Multi-class classification
   - Multi-label classification
2. **Binary logistic regression**
   - Probability estimation
   - Cost and Gradient
   - Gradient (derivation)
   - Parameters' update
3. **Multi-class logistic regression**
   - One-vs-Rest
   - One-vs-One
   - Multinomial
4. **Multi-label logistic regression**
   - Binary relevance
   - Label powerset

Section 1

Classification

Machine Learning

Classification

Classification

Binary

- Classes: 1
- Choice: 1

Multi-class

One-Output

- Classes: L >= 2
- Choice: 1

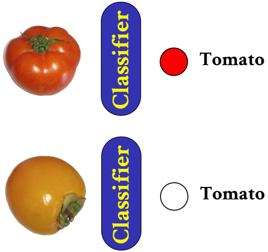
Multi-label

- Classes: L >= 2
- Choice: 0 <= K <= L

Machine Learning: Classification

Binary classification

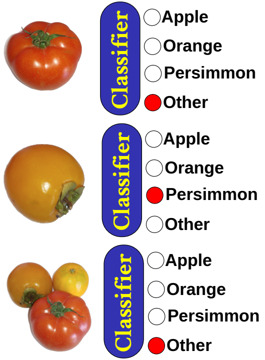
- Number of available classes: 2 (Actually, it is just one class. We test if a sample belongs to it or not)
- Number of chosen classes: 1
- Examples
  - Classify an image as containing a specific object or not.
  - Finding out if a message is a spam or not.



Machine Learning: Classification

Multi-class classification

- Number of available classes: L $\geq$ 2
- Number of chosen classes: 1
- Examples
  - Detect an animal from an input image.
  - Detect a movie's certification (PG, R, etc.) from its description.



Machine Learning: Classification

Multi-class classification: Methods

Multi-class with one output

Generalization

Adapt algorithms to accept multiple classes.
Naive bayes and decision trees are multi-class by default.
Logistic regression: using softmax with a generalized loss function.

Using binary models

One-vs-Rest

Train L binary models.
Each is trained on its samples vs the rest of samples.
To estimate the class, use the most probable one (Argmax)

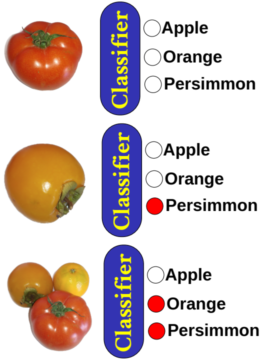
One-vs-One

Train L*(L-1)/2 binary models.
Each is trained on its samples vs another class's samples.
To estimate the class, use the majority vote

Machine Learning: Classification

Multi-label classification

- Number of available classes: $L \geq 2$
- Number of chosen classes: $K \leq L$
- Examples
    - Detect many animals from an input image.
    - Find the clothes (hat, jeans, scarf, etc.) from an image.
    - Detect movie's genres (Sci-fi, Action, Comedy, etc.) from its description.



Machine Learning: Classification

Multi-label classification: Methods [Madjarov et al., 2012]

Multi-label				
Algorithm adaptation	Algorithm transformation			Ensemble based
	Binary relevance	Pair-wise	Label powerset	
Adapt algorithms to accept multiple labels. For example decision trees can be modified to accept many classes in the leafs.	OvR classifiers each estimates a class apart	OvR classifiers using cumulated votes to decide relevant classes	Multi-class with all combinations as classes	Like ensemble methods but using a threshold over cumulative votes to select a class

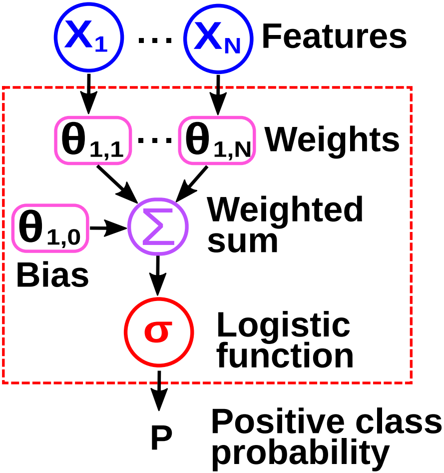
- scikit-multilearn: http://scikit.ml/

Section 2

Binary logistic regression

Machine Learning

Binary logistic regression



Machine Learning: Binary logistic regression

Probability estimation

$$Z = \sum_{j=1}^{N} \theta_j X_j = X \cdot \theta$$

- $Z[M]$ is a vector of M elements (samples)
- $X[M, N]$ is a matrix of M samples and N features
- $\theta[N]$ is a vector of N parameters (weights)

$$H = \sigma(Z) = \frac{1}{1 + e^{-Z}}$$

- $H[M]$ is a vector of M probabilities (samples)

Machine Learning: Binary logistic regression

Cost and Gradient

$$J_\theta = BCE = \frac{-1}{M} \sum_{i=1}^{M} [Y^{(i)} \log(H^{(i)}) + (1 - Y^{(i)}) \log(1 - H^{(i)})]$$

- $Y[M]$ and $H[M]$ are two vectors of M elements (samples)
- J_θ is a scalar

$$\frac{\partial BCE}{\partial \theta_j} = \frac{1}{M} \sum_{i=1}^{M} (H^{(i)} - Y^{(i)}) X_j^{(i)}$$

$$\frac{\partial BCE}{\partial \theta} = \frac{1}{M} (H - Y) \cdot X$$

- $\frac{\partial BCE}{\partial \theta}[N]$ is a vector of N elements (features)

Machine Learning: Binary logistic regression

Gradient (derivation)

$$\begin{aligned}
\frac{\partial BCE}{\partial \theta_j} &= \frac{-1}{M}\sum_{i=1}^{M}\frac{\partial}{\partial \theta_j}[Y^{(i)}\log(H^{(i)}) + (1-Y^{(i)})\log(1-H^{(i)})] \\
&= \frac{-1}{M}\sum_{i=1}^{M}[Y^{(i)}\frac{\partial}{\partial \theta_j}\log(H^{(i)}) + (1-Y^{(i)})\frac{\partial}{\partial \theta_j}\log(1-H^{(i)})] \\
&= \frac{-1}{M}\sum_{i=1}^{M}[Y^{(i)}\frac{1}{H^{(i)}}\frac{\partial}{\partial \theta_j}H^{(i)} + (1-Y^{(i)})\frac{-1}{1-H^{(i)}}\frac{\partial}{\partial \theta_j}H^{(i)})] \\
&= \frac{-1}{M}\sum_{i=1}^{M}\frac{Y^{(i)}-H^{(i)}}{H^{(i)}(1-H^{(i)})}\frac{\partial}{\partial \theta_j}H^{(i)}
\end{aligned}$$

$$\frac{\partial H^{(i)}}{\partial \theta_j} = \frac{\partial \sigma(Z^{(i)})}{\partial Z^{(i)}}\frac{\partial Z^{(i)}}{\partial \theta_j} = [\sigma(Z^{(i)})(1-\sigma(Z^{(i)}))]\frac{\partial}{\partial \theta_j}\sum_{k=0}^{N}\theta_k X_k^{(i)} = H^{(i)}(1-H^{(i)})X_j^{(i)}$$

$$\begin{aligned}
\frac{\partial BCE}{\partial \theta_j} &= \frac{-1}{M}\sum_{i=1}^{M}\frac{Y^{(i)}-H^{(i)}}{H^{(i)}(1-H^{(i)})}[H^{(i)}(1-H^{(i)})X_j^{(i)}] \\
&= \frac{1}{M}\sum_{i=1}^{M}(H^{(i)}-Y^{(i)})X_j^{(i)}
\end{aligned}$$

Machine Learning: Binary logistic regression

Parameters' update

$$\theta = \theta - \alpha \frac{\partial J_\theta}{\partial \theta}$$

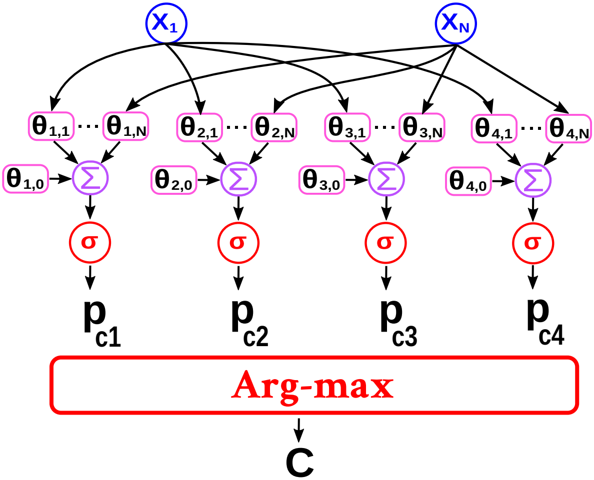
- $\frac{\partial J_\theta}{\partial \theta}[N]$ is a vector of N elements (features)
- $\theta[N]$ is a vector of N elements (features)
- α is a learning rate

Section 3

Multi-class logistic regression

Machine Learning: Multi-class logistic regression

One-vs-Rest



Machine Learning: Multi-class logistic regression

One-vs-Rest: Description

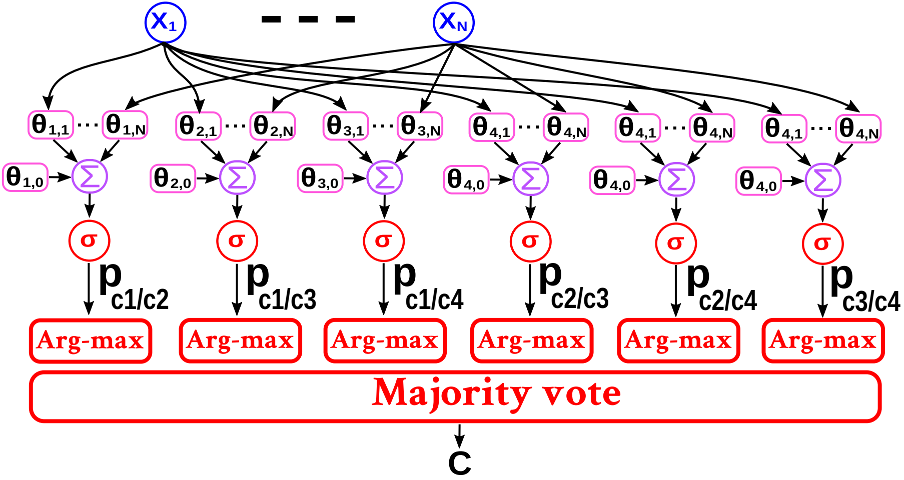
Given L output classes:

- Training
  - For each class C_l, we train a binary model M_l separately
  - In this case, we will have L binary models
  - The positive class is represented by C_l class's samples
  - The negative class is represented by the rest of the samples
- Estimation
  - Given a sample
  - For each class C_l, we estimate its probability using M_l
  - We take the class with the maximum probability
  - In this case, the sum of probabilities does not always give 1

$$\sum_{l=1}^{L} P(l|x; \theta^{M_l}) \in [0, L]$$

Machine Learning: Multi-class logistic regression

One-vs-One



Machine Learning: Multi-class logistic regression

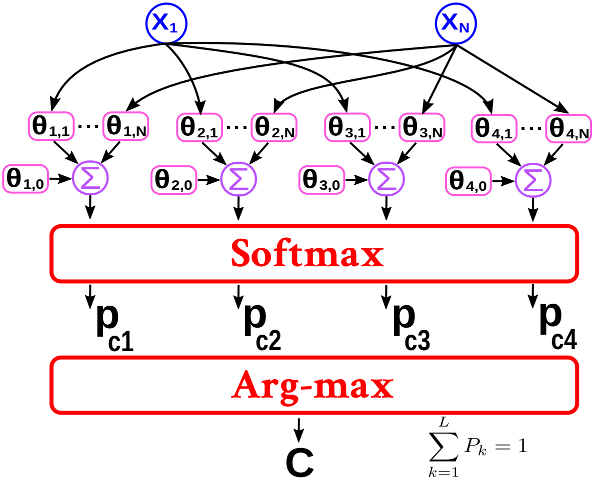
One-vs-One: Description

Given L output classes:

- Training
  - For each two classes C_l and $C_{l'}$, we train a binary model $M_{ll'}$ separately
  - In this case, we will have $L(L-1)/2$ binary models
  - The positive class is represented one of the two classes
  - The negative class is represented by the other class
- Estimation
  - Given a sample
  - For each model $C_{ll'}$, we estimate a probability
  - In this case, the class is either l or l'
  - We count the number of each class being estimated
  - The majority wins (vote)

Machine Learning: Multi-class logistic regression

Multinomial



$$\sum_{k=1}^{L} P_k = 1$$

Machine Learning: Multi-class logistic regression

Multinomial: Description

Given L output classes:

- This is a generalization of binary classification in logistic regression
- Training
  - For each class C_l, we calculate a weighted sum
  - We apply **Softmax** function on these outputs
  - It is a function which transforms the sums into probabilities
  - Also, it normalizes these probabilities to get a sum of 1
  - The output classes are represented using One-Hot
  - The cost function is a generalized version of that of binary classification
- Estimation
  - Given a sample
  - We apply the model to get a vector of probabilities
  - The most probable class wins

Machine Learning: Multi-class logistic regression

Multinomial: Probability estimation

$$Z = \sum_{j=1}^{N} \theta_j X_j = X \cdot \theta$$

- $Z[M, L]$ is a matrix of M samples and L classes
- $X[M, N]$ is a matrix of M samples and N features
- $\theta[N, L]$ is a matrix of N features and L classes

$$H = softmax(Z) = \frac{e^Z}{\sum_{k=1}^{L} e^{Z_k}}$$

- $H[M, L]$ is a matrix of M samples and L classes

Machine Learning: Multi-class logistic regression

Multinomial: Cost and gradient

$$J_\theta = \frac{-1}{M} \sum_{i=1}^{M} \sum_{k=1}^{L} Y_k^{(i)} \log(H_k^{(i)})$$

- $Y[M, L]$ and $H[M, L]$ are two matrices of $M \times L$ elements (features X classes)
- J_θ is a scalar

$$\frac{\partial BCE}{\partial \theta_j} = \frac{1}{M} \sum_{i=1}^{M} (H^{(i)} - Y^{(i)}) X_j^{(i)}$$

$$\frac{\partial BCE}{\partial \theta} = \frac{1}{M} (H - Y) \cdot X$$

- $\frac{\partial BCE}{\partial \theta}[N, L]$ is a matrix of $N \times L$ elements (features X classes)

Machine Learning: Multi-class logistic regression

Multinomial: Parameters' update

$$\theta = \theta - \alpha \frac{\partial J_\theta}{\partial \theta}$$

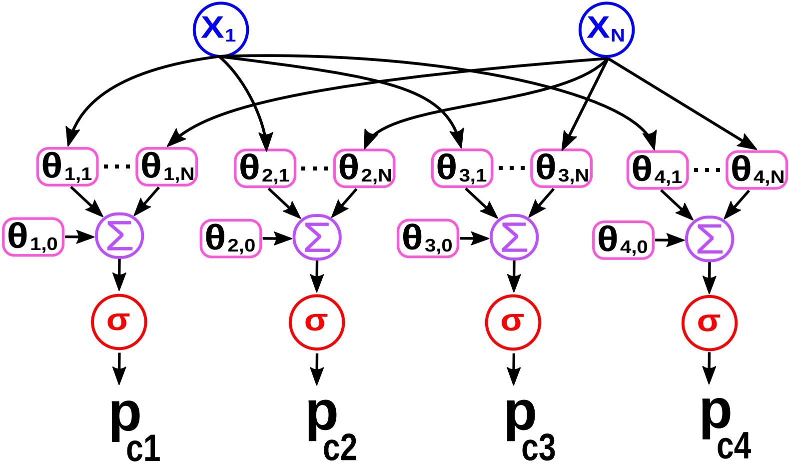
- $\frac{\partial BCE}{\partial \theta}[N, L]$ is a matrix of $N \times L$ elements (features X classes)
- $\theta[N, L]$ is a matrix of N features and L classes
- α is the learning rate

Section 4

Multi-label logistic regression

Machine Learning: Multi-label logistic regression

Binary relevance



Machine Learning: Multi-class logistic regression

Binary relevance: Description

Given L output classes:

- Training
  - For each class C_l, we train a binary model M_l separately
  - In this case, we will have L binary models
  - The positive class is represented by C_l class's samples
  - The negative class is represented by the rest of the samples
- Estimation
  - Given a sample
  - For each class C_l, we estimate its probability using M_l
  - If the probability is greater or equals 50%, then the sample belongs to the class C_l

Machine Learning: Multi-label logistic regression

Label powerset

Dataset with 3 classes (c1, c2, c3) plus other (o)

Samples o	Samples c1	Samples c1+c2	Samples c1+c2+c3
Samples c3	Samples c2	Samples c1+c3	Samples c2+c3

Multi-class classification

(select one of the 8 classes "combinations")

↓

C

Machine Learning: Multi-class logistic regression

Label powerset: Description

Given L output classes:

- Training
  - We look for all combinations of classes
  - Each combination is considered as a new class
  - We train a multi-class model
- Estimation
  - Given a sample
  - We use our trained multi-class model to get one class
  - This class is a combination of many original classes

Section 5

Bibliography

Bibliography

Madjarov, G., Kocev, D., Gjorgjevikj, D., and Džeroski, S. (2012).
An extensive experimental comparison of methods for multi-label learning.
Pattern Recognition, 45(9):3084–3104.
Best Papers of Iberian Conference on Pattern Recognition and Image Analysis (IbPRIA'2011).