Multiclass Classification

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Slides based on Lecture 09 from David Rosenberg's course materials
(https://github.com/davidrosenberg/mlcourse)

CDS, NYU

March 29, 2022

Logistics

Office hour moved to Wed 5:00-6:00pm

Overview

Motivation

- So far, most algorithms we've learned are designed for binary classification.
- Many real-world problems have more than two classes.
- What are some potential issues when we have a large number of classes?

Today's lecture

- How to *reduce* multiclass classification to binary classification?
- How do we *generalize* binary classification algorithm to the multiclass setting?
- Example of very large output space: structured prediction.

Reduction to Binary Classification

One-vs-All / One-vs-Rest

Setting

- Input space: $\mathcal{X}$
- Output space: $\mathcal{Y} = \{1, \ldots, k\}$

Training

- Train k binary classifiers, one for each class: $h_1, \ldots, h_k : \mathcal{X} \to \mathrm{R}$.
- Classifier h_i distinguishes class i (+1) from the rest (-1).

Prediction

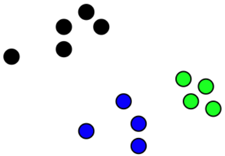
- Majority vote:

$$h(x) = \underset{i \in \{1, \ldots, k\}}{\arg\max}\, h_i(x)$$

- Ties can be broken arbitrarily.

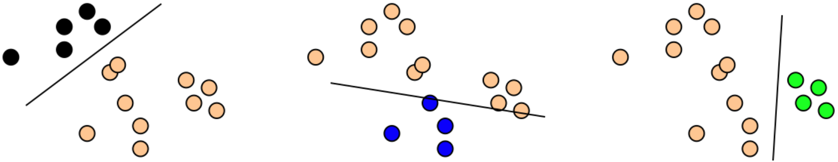
OvA: 3-class example

Consider a dataset with three classes:



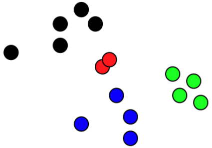
Assumption: each class is linearly separable from the rest.
Ideal case: only target class has positive score.

Train OvA classifiers:



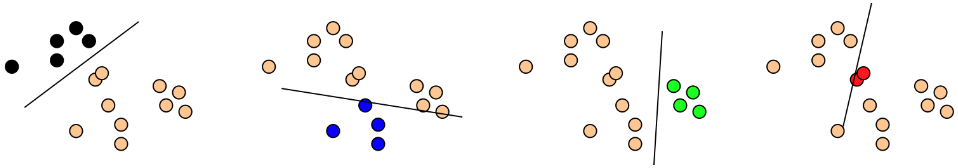
OvA: 4-class non-separable example

Consider a dataset with four classes:



Cannot separate red points from the rest.
Which classes might have low accuracy?

Train OvA classifiers:



All vs All / One vs One / All pairs

Setting

- Input space: $\mathcal{X}$
- Output space: $\mathcal{Y} = \{1, \ldots, k\}$

Training

- Train $\binom{k}{2}$ binary classifiers, one for each pair: $h_{ij} : \mathcal{X} \to \mathrm{R}$ for $i \in [1, k]$ and $j \in [i+1, k]$.
- Classifier h_{ij} distinguishes class i (+1) from class j (-1).

Prediction

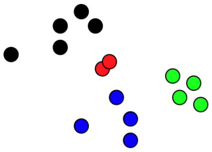
- Majority vote (each class gets $k-1$ votes)

$$h(x) = \underset{i \in \{1, \ldots, k\}}{\arg\max} \sum_{j \neq i} \underbrace{h_{ij}(x)\mathbb{I}\{i < j\}}_{\text{class } i \text{ is } +1} - \underbrace{h_{ji}(x)\mathbb{I}\{j < i\}}_{\text{class } i \text{ is -1}}$$

- Tournament
- Ties can be broken arbitrarily.

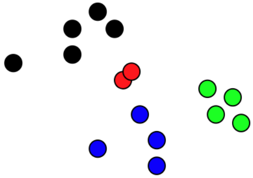
AvA: four-class example

Consider a dataset with four classes:



Assumption: each pair of classes are linearly separable.
More expressive than OvA.

What's the decision region for the red class?



OvA vs AvA

		OvA	AvA
computation	train	$O(kB_{\text{train}}(n))$	$O(k^2B_{\text{train}}(n/k))$
	test	$O(kB_{\text{test}})$	$O(k^2B_{\text{test}})$
challenges	train	class imbalance	small training set
	test	calibration / scale tie breaking	

Lack theoretical justification but simple to implement and works well in practice (when # classes is small).

Review

Reduction-based approaches:

- Reducing multiclass classification to binary classification: OvA, AvA
- Key is to design "natural" binary classification problems without large computation cost.

But,

- Unclear how to generalize to extremely large # of classes.
- ImageNet: >20k labels; Wikipedia: >1M categories.

Next, generalize previous algorithms to multiclass settings.

Multiclass loss

OvA revisit

- **Base Hypothesis Space**: $\mathcal{H} = \{h : \mathcal{X} \to \mathrm{R}\}$ (score functions).
- **Multiclass Hypothesis Space** (for k classes):

$$\mathcal{F} = \left\{ x \mapsto \arg\max_i h_i(x) \mid h_1, \ldots, h_k \in \mathcal{H} \right\}$$

- Intuitively, $h_i(x)$ scores how likely x is to be from class i.
- OvA objective: $h_i(x) > 0$ for x with label i and $h_i(x) < 0$ for x with all other labels.
- At test time, to predict (x, i) correctly we only need

$$h_i(x) > h_j(x) \qquad \forall j \neq i. \tag{1}$$

Multiclass perceptron

- Base linear predictors: $h_i(x) = w_i^T x$ ($w \in \mathrm{R}^d$).
- Multiclass perceptron:

  Given a multiclass dataset $\mathcal{D} = \{(x, y)\}$;
  Initialize $w \leftarrow 0$;
  for $iter = 1, 2, \ldots, T$ **do**
      for $(x, y) \in \mathcal{D}$ **do**
          $\hat{y} = \arg\max_{y' \in \mathcal{Y}} w_{y'}^T x$;
          if $\hat{y} \neq y$ **then** `// We've made a mistake`
              $w_y \leftarrow w_y + x$; `// Move the target-class scorer towards` x
              $w_{\hat{y}} \leftarrow w_{\hat{y}} - x$; `// Move the wrong-class scorer away from` x
          end
      end
  end

Rewrite the scoring function

- Remember that we want to scale to very large # of classes and reuse algorithms and analysis for binary classification
  - $\implies$ a single weight vector is desired
- How to rewrite the equation such that we have one w instead of k?

$$w_i^T x = w^T \psi(x, i) \tag{2}$$
$$h_i(x) = h(x, i) \tag{3}$$

  - Encode labels in the feature space.
  - Score for each label $\rightarrow$ score for the "*compatibility*" of a label and an input.

The Multivector Construction

How to construct the feature map ψ?

- What if we stack w_i's together (e.g., $x \in \mathrm{R}^2, \mathcal{Y} = \{1,2,3\}$)

$$w = \left(\underbrace{-\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}}_{w_1}, \underbrace{0, 1}_{w_2}, \underbrace{\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}}_{w_3} \right)$$

- And then do the following: $\Psi : \mathrm{R}^2 \times \{1,2,3\} \to \mathrm{R}^6$ defined by

$$\begin{aligned} \Psi(x,1) &:= (x_1, x_2, 0, 0, 0, 0) \\ \Psi(x,2) &:= (0, 0, x_1, x_2, 0, 0) \\ \Psi(x,3) &:= (0, 0, 0, 0, x_1, x_2) \end{aligned}$$

- Then $\langle w, \Psi(x,y) \rangle = \langle w_y, x \rangle$, which is what we want.

Rewrite multiclass perceptron

Multiclass perceptron using the multivector construction.

Given a multiclass dataset $\mathcal{D} = \{(x, y)\}$;
Initialize $w \leftarrow 0$;
for $iter = 1, 2, \ldots, T$ **do**
  for $(x, y) \in \mathcal{D}$ **do**
    $\hat{y} = \arg\max_{y' \in \mathcal{Y}} w^T \psi(x, y')$; `// Equivalent to` $\arg\max_{y' \in \mathcal{Y}} w_{y'}^T x$
    if $\hat{y} \neq y$ **then** `// We've made a mistake`
      $w \leftarrow w + \psi(x, y)$; `// Move the scorer towards` $\psi(x, y)$
      $w \leftarrow w - \psi(x, \hat{y})$; `// Move the scorer away from` $\psi(x, \hat{y})$
    end
  end
end

Exercise: What is the base binary classification problem in multiclass perceptron?

Features

Toy multiclass example: Part-of-speech classification

- $\mathcal{X} = \{\text{All possible words}\}$
- $\mathcal{Y} = \{\text{NOUN,VERB,ADJECTIVE}, \ldots\}$.
- Features of $x \in \mathcal{X}$: [The word itself], ENDS_IN_ly, ENDS_IN_ness, ...

How to construct the feature vector?

- Multivector construction: $w \in \mathrm{R}^{d \times k}$—doesn't scale.
- Directly design features for each class.

$$\Psi(x, y) = (\psi_1(x, y), \psi_2(x, y), \psi_3(x, y), \ldots, \psi_d(x, y)) \tag{4}$$

  - Size can be bounded by d.

Features

Sample training data:

```
The boy grabbed the apple and ran away quickly .
```

Feature:

$$
\begin{aligned}
\psi_1(x,y) &= 1(x = \text{apple AND } y = \text{NOUN}) \\
\psi_2(x,y) &= 1(x = \text{run AND } y = \text{NOUN}) \\
\psi_3(x,y) &= 1(x = \text{run AND } y = \text{VERB}) \\
\psi_4(x,y) &= 1(x \text{ ENDS\_IN\_ly AND } y = \text{ADVERB}) \\
&\ldots
\end{aligned}
$$

- E.g., $\Psi(x = \text{run}, y = \text{NOUN}) = (0, 1, 0, 0, \ldots)$
- After training, what's w_1, w_2, w_3, w_4?
- No need to include features unseen in training data.

Feature templates: implementation

- Flexible, e.g., neighboring words, suffix/prefix.
- "Read off" features from the training data.
- Often sparse—efficient in practice, e.g., NLP problems.
- Can use a hash function: template $\rightarrow \{1, 2, \ldots, d\}$.

Review

Ingredients in multiclass classification:

- Scoring functions for each class (similar to ranking).
- Represent labels in the input space $\implies$ single weight vector.

We've seen

- How to generalize the perceptron algorithm to multiclass setting.
- Very simple idea. Was popular in NLP for structured prediction (e.g., tagging, parsing).

Next,

- How to generalize SVM to the multiclass setting.
- Concept check: Why might one prefer SVM / perceptron?

Margin for Multiclass

Binary

- Margin for $(x^{(n)}, y^{(n)})$:

$$y^{(n)} w^T x^{(n)} \tag{5}$$

- Want margin to be large and positive ($w^T x^{(n)}$ has same sign as $y^{(n)}$)

Multiclass

- Class-specific margin for $(x^{(n)}, y^{(n)})$:

$$h(x^{(n)}, y^{(n)}) - h(x^{(n)}, y). \tag{6}$$

- Difference between scores of the correct class and each other class
- Want margin to be large and positive for all $y \neq y^{(n)}$.

Multiclass SVM: separable case

Binary

$$\min_{w} \quad \frac{1}{2}\|w\|^2 \tag{7}$$

$$\text{s.t.} \quad \underbrace{y^{(n)} w^T x^{(n)}}_{\text{margin}} \geqslant 1 \quad \forall (x^{(n)}, y^{(n)}) \in \mathcal{D} \tag{8}$$

Multiclass As in the binary case, take 1 as our target margin.

$$m_{n,y}(w) \stackrel{\text{def}}{=} \underbrace{\left\langle w, \Psi(x^{(n)}, y^{(n)}) \right\rangle}_{\text{score of correct class}} - \underbrace{\left\langle w, \Psi(x^{(n)}, y) \right\rangle}_{\text{score of other class}} \tag{9}$$

$$\min_{w} \quad \frac{1}{2}\|w\|^2 \tag{10}$$

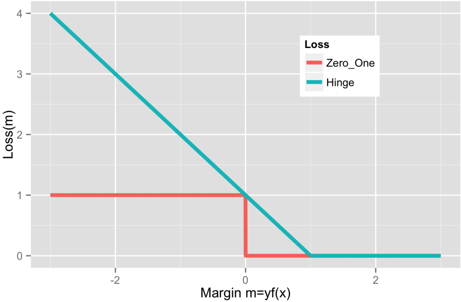
$$\text{s.t.} \quad m_{n,y}(w) \geqslant 1 \quad \forall (x^{(n)}, y^{(n)}) \in \mathcal{D}, y \neq y^{(n)} \tag{11}$$

Exercise: write the objective for the non-separable case

Recap: hingle loss for binary classification

- Hinge loss: a convex upperbound on the 0-1 loss

$$\ell_{\text{hinge}}(y, \hat{y}) = \max(0, 1 - yh(x)) \tag{12}$$



Generalized hinge loss

- What's the zero-one loss for multiclass classification?

$$\Delta(y, y') = \mathbb{I}\{y \neq y'\} \tag{13}$$

- In general, can also have different cost for each class.
- Upper bound on $\Delta(y, y')$.

$$\hat{y} \stackrel{\text{def}}{=} \operatorname*{arg\,max}_{y' \in \mathcal{Y}} \left\langle w, \Psi(x, y') \right\rangle \tag{14}$$

$$\implies \langle w, \Psi(x, y) \rangle \leqslant \langle w, \Psi(x, \hat{y}) \rangle \tag{15}$$

$$\implies \Delta(y, \hat{y}) \leqslant \Delta(y, \hat{y}) - \langle w, (\Psi(x, y) - \Psi(x, \hat{y})) \rangle \qquad \text{When are they equal?} \tag{16}$$

- Generalized hinge loss:

$$\ell_{\text{hinge}}(y, x, w) \stackrel{\text{def}}{=} \max_{y' \in \mathcal{Y}} \left(\Delta(y, y') - \left\langle w, \left(\Psi(x, y) - \Psi(x, y') \right) \right\rangle \right) \tag{17}$$

Multiclass SVM with Hinge Loss

- Recall the hinge loss formulation for binary SVM (without the bias term):

$$\min_{w \in \mathbb{R}^d} \frac{1}{2}||w||^2 + C \sum_{n=1}^{N} \max\left(0, 1 - \underbrace{y^{(n)} w^T x^{(n)}}_{\text{margin}}\right).$$

- The multiclass objective:

$$\min_{w \in \mathbb{R}^d} \frac{1}{2}||w||^2 + C \sum_{n=1}^{N} \max_{y' \in \mathcal{Y}} \left(\Delta(y, y') - \underbrace{\langle w, (\Psi(x, y) - \Psi(x, y')) \rangle}_{\text{margin}}\right)$$

  - $\Delta(y, y')$ as target margin for each class.
  - If margin $m_{n,y'}(w)$ meets or exceeds its target $\Delta(y^{(n)}, y')$ $\forall y \in \mathcal{Y}$, then no loss on example n.

Recap: What Have We Got?

- Problem: Multiclass classification $\mathcal{Y} = \{1, \ldots, k\}$
- Solution 1: One-vs-All
  - Train k models: $h_1(x), \ldots, h_k(x) : \mathcal{X} \to \mathrm{R}$.
  - Predict with $\arg\max_{y \in \mathcal{Y}} h_y(x)$.
  - Gave simple example where this fails for linear classifiers
- Solution 2: Multiclass loss
  - Train one model: $h(x, y) : \mathcal{X} \times \mathcal{Y} \to \mathrm{R}$.
  - Prediction involves solving $\arg\max_{y \in \mathcal{Y}} h(x, y)$.

Does it work better in practice?

- Paper by Rifkin & Klautau: "In Defense of One-Vs-All Classification" (2004)
  - Extensive experiments, carefully done
    - albeit on relatively small UCI datasets
  - Suggests one-vs-all works just as well in practice
    - (or at least, the advantages claimed by earlier papers for multiclass methods were not compelling)
- Compared
  - many multiclass frameworks (including the one we discuss)
  - one-vs-all for SVMs with RBF kernel
  - one-vs-all for square loss with RBF kernel (for classification!)
- All performed roughly the same

Why Are We Bothering with Multiclass?

- The framework we have developed for multiclass
  - compatibility features / scoring functions
  - multiclass margin
  - target margin / multiclass loss
- Generalizes to situations where k is very large and one-vs-all is intractable.
- Key idea is that we can generalize across outputs y by using features of y.

Introduction to Structured Prediction

Example: Part-of-speech (POS) Tagging

- Given a sentence, give a part of speech tag for each word:

x	$\underbrace{\text{[START]}}_{x_0}$	$\underbrace{\text{He}}_{x_1}$	$\underbrace{\text{eats}}_{x_2}$	$\underbrace{\text{apples}}_{x_3}$
y	$\underbrace{\text{[START]}}_{y_0}$	$\underbrace{\text{Pronoun}}_{y_1}$	$\underbrace{\text{Verb}}_{y_2}$	$\underbrace{\text{Noun}}_{y_3}$

- $\mathcal{V} = \{\text{all English words}\} \cup \{\text{[START]}, ”.”\}$
- $\mathcal{X} = \mathcal{V}^n$, $n = 1, 2, 3, \ldots$ [Word sequences of any length]
- $\mathcal{P} = \{\text{START}, \text{Pronoun}, \text{Verb}, \text{Noun}, \text{Adjective}\}$
- $\mathcal{Y} = \mathcal{P}^n$, $n = 1, 2, 3, \ldots$[Part of speech sequence of any length]

Multiclass Hypothesis Space

- Discrete output space: $\mathcal{Y}(x)$
  - Very large but has structure, e.g., linear chain (sequence labeling), tree (parsing)
  - Size depends on input x
- Base Hypothesis Space: $\mathcal{H} = \{h : \mathcal{X} \times \mathcal{Y} \to \mathrm{R}\}$
  - $h(x, y)$ gives compatibility score between input x and output y
- Multiclass hypothesis space

$$\mathcal{F} = \left\{ x \mapsto \arg\max_{y \in \mathcal{Y}} h(x, y) \mid h \in \mathcal{H} \right\}$$

- Final prediction function is an $f \in \mathcal{F}$.
- For each $f \in \mathcal{F}$ there is an underlying compatibility score function $h \in \mathcal{H}$.

Structured Prediction

- Part-of-speech tagging

$x:$	he	eats	apples
$y:$	pronoun	verb	noun

- Multiclass hypothesis space:

$$h(x,y) = w^T\Psi(x,y) \tag{18}$$

$$\mathcal{F} = \left\{ x \mapsto \arg\max_{y\in\mathcal{Y}} h(x,y) \mid h \in \mathcal{H} \right\} \tag{19}$$

- A special case of multiclass classification
- How to design the feature map Ψ? What are the considerations?

Unary features

- A **unary feature** only depends on
  - the label at a single position, y_i, and x
- Example:

$$
\begin{aligned}
\phi_1(x, y_i) &= 1(x_i = \text{runs})1(y_i = \text{Verb}) \\
\phi_2(x, y_i) &= 1(x_i = \text{runs})1(y_i = \text{Noun}) \\
\phi_3(x, y_i) &= 1(x_{i-1} = \text{He})1(x_i = \text{runs})1(y_i = \text{Verb})
\end{aligned}
$$

Markov features

- A **markov feature** only depends on
  - two adjacent labels, y_{i-1} and y_i, and x
- Example:

$$\begin{aligned}\theta_1(x, y_{i-1}, y_i) &= 1(y_{i-1} = \text{Pronoun})1(y_i = \text{Verb}) \\ \theta_2(x, y_{i-1}, y_i) &= 1(y_{i-1} = \text{Pronoun})1(y_i = \text{Noun})\end{aligned}$$

- Reminiscent of Markov models in the output space
- Possible to have higher-order features

Local Feature Vector and Compatibility Score

- At each position i in sequence, define the **local feature vector** (unary and markov):

$$\begin{aligned}\Psi_i(x, y_{i-1}, y_i) &= (\phi_1(x, y_i), \phi_2(x, y_i), \ldots, \\ &\quad \theta_1(x, y_{i-1}, y_i), \theta_2(x, y_{i-1}, y_i), \ldots)\end{aligned}$$

- And **local compatibility score** at position i: $\langle w, \Psi_i(x, y_{i-1}, y_i)\rangle$.

- The compatibility score for (x, y) is the sum of local compatibility scores:

$$\sum_i \langle w, \Psi_i(x, y_{i-1}, y_i)\rangle = \left\langle w, \sum_i \Psi_i(x, y_{i-1}, y_i)\right\rangle = \langle w, \Psi(x, y)\rangle, \tag{20}$$

where we define the **sequence feature vector** by

$$\Psi(x, y) = \sum_i \Psi_i(x, y_{i-1}, y_i). \qquad \text{decomposable}$$

Structured perceptron

Given a dataset $\mathcal{D} = \{(x, y)\}$;
Initialize $w \leftarrow 0$;
for $iter = 1, 2, \ldots, T$ **do**
    for $(x, y) \in \mathcal{D}$ **do**
        $\hat{y} = \arg\max_{y' \in \mathcal{Y}(x)} w^T \psi(x, y')$;
        if $\hat{y} \neq y$ **then** `// We've made a mistake`
            $w \leftarrow w + \Psi(x, y)$; `// Move the scorer towards` $\psi(x, y)$
            $w \leftarrow w - \Psi(x, \hat{y})$; `// Move the scorer away from` $\psi(x, \hat{y})$
        end
    end
end

Identical to the multiclass perceptron algorithm except the $\arg\max$ is now over the structured output space $\mathcal{Y}(x)$.

Structured hinge loss

- Recall the generalized hinge loss

$$\ell_{\text{hinge}}(y, \hat{y}) \stackrel{\text{def}}{=} \max_{y' \in \mathcal{Y}(x)} \left(\Delta(y, y') + \left\langle w, \left(\Psi(x, y') - \Psi(x, y) \right) \right\rangle \right) \tag{21}$$

- What is $\Delta(y, y')$ for two sequences?
- **Hamming loss** is common:

$$\Delta(y, y') = \frac{1}{L} \sum_{i=1}^{L} 1(y_i \neq y_i')$$

where L is the sequence length.

Structured SVM

Exercise:

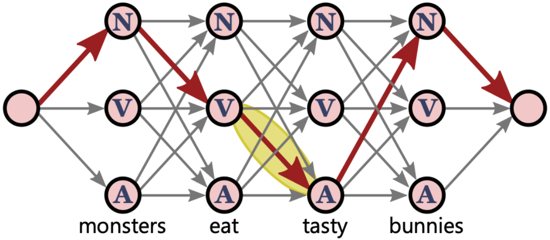
- Write down the objective of structured SVM using the structured hinge loss.
- Stochastic sub-gradient descent for structured SVM (similar to HW3 P3)
- Compare with the structured perceptron algorithm

The argmax problem for sequences

Problem To compute predictions, we need to find $\arg\max_{y \in \mathcal{Y}(x)} \langle w, \Psi(x, y) \rangle$, and $|\mathcal{Y}(x)|$ is exponentially large.

Observation $\Psi(x, y)$ decomposes to $\sum_i \Psi_i(x, y)$.

Solution Dynamic programming (similar to the Viterbi algorithm)



What's the running time?

Figure by Daumé III. A course in machine learning. Figure 17.1.

The argmax problem in general

Efficient problem-specific algorithms:

problem	structure	algorithm
constituent parsing	binary trees with context-free features	CYK
dependency parsing	spanning trees with edge features	Chu-Liu-Edmonds
image segmentation	2d with adjacent-pixel features	graph cuts

General algorithm:

- Integer linear programming (ILP)

$$\max_z a^T z \quad \text{s.t. linear constraints on } z \tag{22}$$

- z: indicator of substructures, e.g., $\mathbb{I}\{y_i = \text{article and } y_{i+1} = \text{noun}\}$
- constraints: z must correspond to a valid structure

Conclusion

Multiclass algorithms

- Reduce to binary classification, e.g., OvA, AvA, ECCO
  - Good enough for simple multiclass problems
- Generalize binary classification algorithms using multiclass loss
  - Useful for problems with extremely large output space, e.g., structured prediction
  - Related problems: ranking, multi-label classification